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#### **Executive Summary**

The Community Surface Dynamic Modeling System (CSDMS) is a NSF-supported, international and community-driven program that seeks to transform the science and practice of earth-surface dynamics modeling. CSDMS, now in its 7th year, integrates a diverse community of 1160 members representing 172 U.S. institutions (126 academic, 25 private, 21 federal) and 292 non-U.S. institutions from 67 countries (190 academic, 30 private, 72 government). There are now 464 affiliated institutions plus another 31 private memberships. CSDMS distributes 228 Open Source models and modeling tools, provides access to high performance computing clusters in support of developing and running models, and offers a suite of products for education and knowledge transfer. The CSDMS architecture employs frameworks and services that convert stand-alone models into flexible "plug-and-play" components to be assembled into larger applications. CSDMS activities are supported through multiple NSF funding units: GEO/OCE Marine Geology and Geophysics, GEO/EAR Geoinformatics; GEO/EAR Geomorphology and Land-use Dynamics; GEO/EAR Sedimentary Geology and Paleontology; GEO/EAR Education and Human Resources; GEO/EAR Hydrological Sciences; BIO/DEB Macrosystems Biology; BIO/DEB Ecosystem Studies. This report highlights the CSDMS Web Modeling Tool (WMT), the web-based successor to the desktop Component Modeling Tool. WMT is a web application that allows users to build and run coupled Earth system models on a high-performance computing cluster (HPCC) from a web browser, web portal developments, and model uncertainty support services. Reports from each of the five CSDMS Working Groups and six Focus Research Groups outline past achievements and their plans to implement the 2013 CSDMS Strategic Plan. This Annual Report covers the period from August 2013 to July 2014.



#### CSDMS 2.0 2014 Annual Report Table of Contents

2.0 CSDMS Management and Oversight42.1 CSDMS Executive Committee (ExCom)42.2 CSDMS Steering Committee (SC)42.3 CSDMS Working and Focus Research Groups52.4 CSDMS Integration Facility (IF)62.5 Industrial Partners62.6 CSDMS Interagency Committee63.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies144.5 CSDMS Portal14
2.2 CSDMS Steering Committee (SC)42.3 CSDMS Working and Focus Research Groups52.4 CSDMS Integration Facility (IF)62.5 Industrial Partners62.6 CSDMS Interagency Committee63.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
2.3 CSDMS Working and Focus Research Groups52.4 CSDMS Integration Facility (IF)62.5 Industrial Partners62.6 CSDMS Interagency Committee63.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
2.4 CSDMS Integration Facility (IF)62.5 Industrial Partners62.6 CSDMS Interagency Committee63.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
2.5 Industrial Partners62.6 CSDMS Interagency Committee63.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
2.6 CSDMS Interagency Committee63.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.0 Just the Facts73.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.1 CSDMS Model Repository73.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.2 CSDMS Data Repository83.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.3 CSDMS Education & Knowledge Transfer (EKT) Repository83.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.4 CSDMS Experimental Supercomputer93.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.5 CSDMS Web Portal Statistics93.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
3.6 CSDMS YouTube Statistics104.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
4.0 CSDMS 2.0 Year 2114.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
4.1 CSDMS Software Stack114.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
4.2 The CSDMS WMT114.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
4.3 Framework Service Components144.4 Semantic Mediation and Ontologies14
4.4 Semantic Mediation and Ontologies 14
4.5 CSDMS Portal 14
4.6 Education and Knowledge Transfer 17
4.7 Educating Model Users and Developers 17
4.8 Advanced Modeling Labs for Graduate and Senior Undergraduate Students 18
4.9 Science on a Sphere Animations 19
4.10 Hands-on Clinics and Courses 19
5.0 Conferences & Publications 21
6.0 CSDMS 2.0: Working & Focus Research Groups
6.1 Terrestrial Working Group 26
6.2 Coastal Working Group 28
6.3 Marine Working Group 29
6.4 Cyberinformatics and Numerics Working Group 30
6.5 Education and Knowledge Transfer Working Group 31
6.6 Carbonate Focus Research Group33
6.7 Hydrology Focus Research Group 34
6.8 Chesapeake Focus Research Group 36
6.9 Geodynamics Focus Research Group 37
6.10 Anthropocene Focus Research Group38
6.11 Critical Zone Focus Research Group40
7.0 CSDMS2.0 Year 3 Priorities and Management of Resources43
7.1 CSDMS2.0 Year 3 Goals — CSDMS Portal 43
7.2 CSDMS2.0 Year 3 Goals — Cyber Plans 44
7.2.1 Supplemental work plan—BMI Builder 44
7.3 CSDMS2.0 Year 3 — EKT Goals 45
8.0 NSF Revenue & Expenditure47
Appendix 1: Institutional Memberships & Member Location Maps 49
Appendix 2: 2014 CSDMS Annual Meeting Abstracts (Keynotes and Posters) 55
Appendix 3: 2014 CSDMS Annual Meeting Clinics 77
Appendix 4: 2014 CSDMS Annual Meeting Awards   81
Appendix 5: CSDMS Special issue: Uncertainty and Sensitivity in Surface Dynamics Modeling     83       Appendix 5: CSDMS Special issue: Uncertainty and Sensitivity in Surface Dynamics Modeling     83
Appendix 6: Towards Improved Uncertainty Quantification for Earth System Models85Appendix 7: Plug and Play Component Modeling- The CSDMS2.0 Approach105

# CSDMS 2.0 2014 Annual Report

# **1.0 CSDMS Mission**

The Community Surface Dynamics Modeling System (CSDMS) catalyzes new paradigms and practices in developing and employing software to understand the earth's surface — the ever-changing dynamic interface between lithosphere, hydrosphere, cryosphere and atmosphere. CSDMS focuses on the movement of fluids and the sediment and solutes they transport through landscapes, seascapes and sedimentary basins. CSDMS supports the development, integration, dissemination and archiving of community open-source software that reflects and predicts earth-surface processes over a broad range of temporal and spatial scales.

# 2.0 CSDMS Management and Oversight

2.1 The CSDMS Executive Committee (ExCom) is comprised of organizational chairpersons:

- Patricia Wiberg (April 2012-), Chair, CSDMS Steering Committee, Univ. of Virginia, VA
- Brad Murray (April 2007—), Chair, Coastal Working Group & Coastal Vulnerability Initiative, Duke Univ., NC
  - Chris Thomas (May 2014 —), Vice Chair, Coastal WG, British Geological Society, Edinburgh, UK
  - Hans-Peter Plag (May 2014—), Vice Chair, Coastal Vulnerability Initiative, Old Dominion U., Norfolk, VA
- Courtney Harris (April 2012—), Chair, Marine WG & Continental Margin Initiative, VIMS, VA
- Greg Tucker (April 2007—), Chair, Terrestrial WG, CIRES, U. Colorado Boulder, CO
- Eckart Meiburg (Jan 2009—), Chair, Cyberinformatics & Numerics WG, U. California-Santa Barbara, CA

- Scott Peckham (Dec. 2013—) Vice Chair, Cyberinformatics & Numerics WG, U. Colorado – Boulder

- Samuel Bentley (Sept. 2012—), Chair, Education & Knowledge Transfer WG, LSU, LA
- Peter Burgess (Sept. 2008—), Chair, Carbonate Focus Research Group, Royal Holloway, U. London, UK
- Carl Friedrichs (April. 2009—), Chair, Chesapeake Focus Research Group, VIMS, VA
- Jonathan Goodall (Nov, 2010—), Chair, Hydrology FRG, U. South Carolina, Columbia SC
- Chris Duffy (Mar. 2013—), Chair, Critical Zone Focus Research Group, Penn State U., PA
- Michael Ellis (Jan. 2013- July 2014), Co-Chair, Anthropocene FRG, British Geol. Survey, UK
- Kathleen Galvin (Jan. 2013—), Co-Chair, Anthropocene FRG, Colorado State U, CO
- Phaedra Upton (Mar. 2013-), Co-Chair, Geodynamics FRG, GNS, New Zealand
- Mark Behn (Mar. 2013—), Co-Chair, Geodynamics Focus Research Group, WHOI, MA
- James Syvitski (ex-officio), CSDMS Executive Director, INSTAAR, University of Colorado Boulder

The Executive Committee is the primary decision-making body of CSDMS, and ensures that the NSF Cooperative Agreement is met, oversees the Bylaws & Operational Procedures, and sets up the annual science plan. The ExCom approves the business reports, management plan, budget, partner memberships, and other issues that arise in the running of CSDMS.

**2.2 The CSDMS Steering Committee (SC)** includes representatives of U.S. Federal Agencies, Industry, and Academia:

- Patricia Wiberg (Sept. 2012—), Chair, CSDMS Steering Committee, Univ. of Virginia, VA
- Tom Drake (April 2007—), U.S. Office of Naval Research, Arlington, VA
- Bert Jagers (April 2007-), Deltares, Delft, The Netherlands
- Marcelo Garcia (Dec. 2012—), Univ. Illinois at Urbana-Champaign, IL

- Chris Paola (Sept. 2009—), NCED, U. Minnesota, Minneapolis, MN
- Cecilia DeLuca (Sept. 2009—), ESMF, NOAA/CIRES, Boulder, CO
- Boyana Norris (Sept. 2009—), University of Oregon, Eugene, OR
- Guillermo Auad (Jan. 2013-), Bureau of Ocean and Energy Management, Herndon, VA
- Martin Perlmutter (Jan. 2014 —), Chevron, Exploration Technology Company, Houston, TX
- James Syvitski (ex-officio), CSDMS Executive Director, INSTAAR, CU-B, Boulder, CO
- **Bilal Haq** (*ex-officio*), National Science Foundation
- Paul Cutler (ex-officio), National Science Foundation

The CSDMS SC assesses the competing objectives and needs of CSDMS, assesses progress in terms of science, outreach and education, advises on revisions to the 5-year strategic plan, and approves the Bylaws and its revisions.

# 2.3 CSDMS Working and Focus Research Groups

There are currently 1160 CSDMS members (58% U.S.) representing 172 U.S. institutions (126 academic, 25 private, 21 federal) and 292 non-U.S. institutions from 67 countries (190 academic, 30 private, 72 government). Members are organized within 5 working groups (Terrestrial, Coastal, Marine, Education and Knowledge Transfer, and Cyberinformatics and Numerics) and 6 focus research groups (Anthropocene, Carbonate, Hydrology, Critical Zone, Geodynamics, and Chesapeake).

Terrestrial	549	Carbonate	73
Coastal	420	Chesapeake	50
Hydrology	410	Critical Zone	27
Marine	279	Anthropocene	25
Cyber	172	Geodynamics	50
EKT	180		



Fig. 1. Growth in active membership (y-axis) per day as of November 2009 (x-axis). CSDMS has 1160 members as of July 15<sup>th</sup>, 2014.

# 2.4 The CSDMS Integration Facility (IF)

The CSDMS Integration Facility (IF) maintains the CSDMS repositories, facilitates community communication and coordination, public relations, and product penetration. The IF develops the CSDMS cyber-infrastructure, provides software guidance to the CSDMS community, maintains the CSDMS vision, and supports cooperation between observational and modeling communities. As of July 2014, CSDMS IF staff includes:

- Executive Director, Prof. James Syvitski (April, 2007-) CSDMS & CU support
- Executive Assistant, Lauren Borkowski (Jan. 2014 -----) CSDMS support
- Senior Software Engineer, Dr. Eric Hutton (April 2007-) CSDMS & other NSF support
- Software Engineer, Dr. Mark Piper (Oct. 2013-) CSDMS & other NSF support
- Cyber Scientist Dr. Albert Kettner (July 2007-) CSDMS & other NSF/NASA support
- EKT Scientist Dr. Irina Overeem (Sept. 2007-) CSDMS & other NSF/NASA support
- Postdoctoral Fellow Kimberly Rogers (March 2012-) Other NSF support
- Ph.D. GRA Stephanie Higgins (Sept. 2010-) NASA support
- Ph.D. GRA Fei Xing (July 2010-) Other NSF support
- Ph.D. GRA Ben Hudson (May 2010-) Other NSF support
- Systems Administrator Chad Stoffel (April 2007-) multiple grant support
- Director Dartmouth Flood Observatory, G Robert Brakenridge (Jan. 2010-) NASA support
- Senior Research Scientist Christopher Jenkins (Jan. 2009-) NSF & other support

#### Departures

• Dr. Scott Peckham (April 2007-July 2013)

# **2.5 CSDMS Industrial Partners**

Industry partners (csdms.colorado.edu/wiki/Industry\_partners) play an important role in contributing to the success of CSDMS through their financial or in-kind contributions. Sponsorship supports the CSDMS effort and thus the next generation of researchers working to develop innovative approaches towards modeling complex earth-surface systems. CSDMS consortium members: 1) demonstrate corporate responsibility and community relations; 2) contribute to the direction of CSDMS research and products; 3) access the latest CSDMS products and information; and 4) join an association of diverse scientists, universities, agencies, and industries. Approximately 12% of CSDMS member institutions are with the private sector.

## 2.6 CSDMS Interagency Committee

This group is comprised of the 21 US agencies (see list in Appendix 1). The committee coordinates their members' collaboration with and support of CSDMS efforts. For 2014, the focus was to appoint a more formal Chair of the Committee. On March 17, 2014, a teleconference regarding this search was held. A meeting to follow up on this search will be held in August 2014. Most agencies rely on models that are developed or are funded in-house for reasons of quality control, specificity, familiarity (with the developers, agency users, and contractors), and cost of changing. Still, the CSDMS community and its products might offer agencies coupled models that these same agencies might like to see developed. In the near term, CSDMS can contribute to understanding of how to build and deploy coupled models. Individual agencies might be "early adopters" and leverage CSDMS to develop coupled models to address specific topics. A task force of the CSDMS Interagency Committee has agreed to explore early adoption strategies.

As a proof of concept, CSDMS is providing help in coupling a high-resolution RANS (Reynolds-averaged Navier-Stokes) turbidity current model (*TURBINS* UCSB) to a coarser resolution (RANS) ocean circulation model ROMS with the Community Surface Transport Model enabled. The project is being funded through a cooperative agreement with the Bureau of Ocean Energy Management (BOEM).

# **3.0 JUST THE FACTS**

# 3.1 CSDMS Model Repository

The CSDMS Model Repository hosts open-source models, modeling tools, and plug-and-play components, including: i) Cryospheric (e.g. glaciers, permafrost, icebergs), ii) Hydrologic, from reach to global scale, iii) Marine (e.g. ocean circulation), iv) River, coastal and estuarine morphodynamics, v) Landscape or seascape evolution, vi) Stratigraphic, and vii) Affiliated domains (e.g. weather & climate models). About 70% of the models are distributed through a central repository; others are distributed through linkages to existing community efforts. Centralized downloads exceed 13000 and redirected download traffic to other sites is similarly high. The 225 projects noted below may involve more than one model.

Repository lines of code statistics as of July 2014: csdms.colorado.edu/wiki/Model\_SLOC\_Page

Language	Projects	Comment	Source
Fortran 77/90/95+	61	1067184	2457617
c/c++	103	367599	1183938
Python	32	87194	140274
C#	1	29344	160373
MATLAB	19	43599	67852
IDL	5	38834	36954
Statistical Analysis Software	1	2390	5796
Java	2	2214	12851
Visual Basic	1	537	8581
Total	225	1638895	4074236

Models, Tools & Components by Environmental Domain http://csdms.colorado.edu/wiki/Main\_Page

Domain	Models	Tools	Components
Terrestrial	81	49	3
Coastal	53	3	4
Marine	44	4	2
Hydrology	54	40	2
Carbonate	3	1	0
Climate	10	2	0

The community models downloaded from other sites (e.g. ROMS, NearCOM, DELT3D) are not counted. The top ten most downloaded models by version as of July 2014 are: (http://csdms.colorado.edu/wiki/Model\_download\_Page)

	Model	No. Times	Торіс
1.	topotoolbox	2212	A set of Matlab functions for topographic analysis
2.	child	1331	Landscape evolution model
3.	topoflow	915	Spatially-distributed, D8-based hydrologic model
4.	hydrotrend	459	Climate driven hydrological transport model
5.	sedflux	447	Basin filling stratigraphic model
6.	2dflowvel	302	Tidal & wind-driven coastal circulation routine
7.	cem	271	Coastal evolution model
8.	bing	268	Submarine debris flows
9.	adi-2d	236	Advection Diffusion Implicit method for 2D diffusion
10.	gc2d	212	Glacier / ice sheet evolution model

#### 3.2 CSDMS Data Repository csdms.colorado.edu/wiki/Data\_download

Data Repository as of July 2014							
Data Type	Databases	Land cover					
Topography/bathy	18	Life Forms	1				
Climate	6	Substrates	4				
Hydrography	6	Human Dimensions	2				
River discharge	8	Sea level	1				
Cryosphere	5	Oceanography	11				
Surface Properties	5	GIS Tools	12				

# 3.3 CSDMS Education & Knowledge Transfer (EKT) Repository

The **Education Repository** offers undergraduate and graduate modeling courses, educational modules, modeling labs, and process and simulation movies.

Animations library csdms.colorado.edu/wiki/Movies\_portal

Environmental Animations	8	Marine Animations	11
Terrestrial Animations	22	Laboratory Movies	14
Coastal Animations	23	Real Event Movies	37
Image Library csdms.colorado.edu/wik	i/Images_portal		
Terrestrial Images	90		
Coastal and Marine Images	49		

#### Modeling Labs csdms.colorado.edu/wiki/Labs\_portal

Modeling Labs are being designed to have a tiered approach. There are spreadsheet labs that emphasize quantitative skills, but address earth surface process questions/problems with reduced parameter space. These labs are focused on undergraduate education and include lesson plans and teacher material. CMT-based modeling labs offer additional complexity, and simulations can be run with more freedom in complexity level. The EKT web pages point to members who have active online teaching resources.

#### Current available labs:

- 1. Glacio-Hydrological Modeling
- 2. River-Delta Interactions
- 3. Sediment Supply to the Global Ocean
- 4. Landscape Evolution Experiments with WILSIM
- 5. Landscape Evolution Modeling with ERODE
- 6. Earth Science Models for K6-12
- 7. Coastal Engineering Experiments

- 8. Hydrological Processes Exercises
- 9. Sinking Deltas
- 10. Stratigraphic Modeling with Sedflux
- 11. Get Started with CMT
- 12. Advanced Use of CMT
- 13. Modeling River Plumes
- 14. Simple Sediment Transport Experiments
- 15. Coastal Stratigraphy Numerical Experiments

#### Modeling Lectures and Courses csdms.colorado.edu/wiki/Lectures\_portal

- 1. Surface Dynamics Modeling with CMT I Overeem & SD Peckham
- 2. Quantitative Earth-surface Dynamics Modeling JPM Syvitski
- 3. 1D Sediment Transport G Parker
- 4. Morphodynamics of Rivers G Parker
- 5. Source to Sink Systems around the World Keynote Chapman Lectures
- 6. Plug and Play Component Technology JPM Syvitski and I Overeem

- 7. Geological Modeling I Overeem
- 8. Deltas: Dynamics, Morphology and Observing of delta processes and human impacts Syvitski

Modeling Textbooks csdms.colorado.edu/wiki/Modeling\_Textbooks

- 1. Mathematical Modeling of Earth's Dynamical Systems By: Slingerland, R., Kump, L.
- 2. Geomorphology; the Mechanics and Chemistry of Landscapes By: Anderson, R., Anderson, S.
- 3. Quantitative Modeling of Earth Surface Processes By: Pelletier, J.D.
- 4. Simulating Clastic Sedimentary Basins: Physical Fundamentals and Computing Procedures By: R.L. Slingerland, K. Furlong and J. Harbaugh
- 5. 1D Sediment Transport Morphodynamics applications to Rivers & Turbidity Currents By: G Parker

# 3.4 CSDMS Experimental Supercomputer <u>csdms.colorado.edu/wiki/HPCC\_information</u>

Approximately 370 individuals now have accounts on the system and have met the use criteria:

- Running a CSDMS model(s) to advance science
- Developing a model that will ultimately become part of the CSDMS model repository.
- Developing a new data systems or visualizations in support of CSDMS models.

The CSDMS High Performance Computing Cluster (HPCC) System *Beach* (Syvitski is PI) is an SGI Altix XE 1300 with 88 compute nodes (704 cores, 3.0 GHz Harpertown processors  $\approx$  8 Tflops). 64 nodes have 16 GB of memory each; 16 nodes have 32 GB of memory each. Internode communication uses a non-blocking InfiniBand fabric. Each compute node has 250 GB of local temporary storage and can access 72TB (raw) of RAID storage through NFS. *Beach* provides GNU and Intel compilers as well as their MPI counterparts (mvapich2, mpich2, and openmpi). *Beach* is supported by the CU ITS Managed Services (UnixOps) under contract to CSDMS. The larger *Janus* supercomputing cluster (Syvitski is Co-PI) consists of 1368 nodes, each containing two 2.8 GHz Intel Westmere processors with six cores each (16,416 cores total) and 24 GB of memory (2 GB/core) per node. Nodes are connected using a non-blocking quad-data rate InfiniBand interconnect, and 1 PB of parallel temporary disk storage. *Beach* is connected to the *Janus* cluster through a private 10 Gb/s network. The system enables *Beach* to quickly share large data sets using the *Janus* 1PB lustre file system. The *Janus* system CU Research Computing manages *Janus*. CPU Utilization rates on *Beach* average 70%.

## 3.5 CSDMS Web Portal Statistics csdms.colorado.edu/wiki/Special:Statistics

Content Pages	1,521	Page Edits	221,416
Total Pages	8,010	Registered Users	1,219
Upload Files	3,175	View Statistics	23,589,385

## 3.6 CSDMS YouTube Statistics http://www.youtube.com/user/CSDMSmovie

CSDMS YouTube channel hosts its (model) animations, laboratory experiments, real events and conference talks. Close to 131 people have now subscribed to the channel to stay informed about new uploads. The channel contains 141 short movies, which in total have been viewed 177,550 times. CSDMS started this channel to make people aware of how illustrative and sophisticated model simulations or associated movies can be. The movies on the CSDMS YouTube channel can be viewed through the CSDMS website: http://csdms.colorado.edu/wiki/Movies\_portal or at http://www.youtube.com/user/CSDMSmovie.

# Top 10 most viewed CSDMS YouTube movies:

Global circulation	63,705	http://www.youtube.com/watch?v=qh011eAYjAA
Laurentide Ice Sheet	13,335	http://www.youtube.com/watch?v=wbsURVgoRD0
Delta formation	7,011	http://www.youtube.com/watch?v=eVTxzuaB00M
World dams since 1800	6,344	http://www.youtube.com/watch?v=OR5IFcSsaxY
Sand Ripples	5,770	http://www.youtube.com/watch?v=rSzGOCo4JEk
Floodplain Evolution	4,552	http://www.youtube.com/watch?v=QqOfP3gVR4s
Spit Evolution	4,358	http://www.youtube.com/watch?v=N_LBeJPWqFM
Barrier Island	3,287	http://www.youtube.com/watch?v=VCX_SzPydsw
Allier river meander	3,093	http://www.youtube.com/watch?v=i0KByNRGv_8
Meandering river	3,019	http://www.youtube.com/watch?v=z3ub6_VwReY



Photo: CSDMS Annual Meeting

# 4.0 CSDMS2.0 Year 2

# 4.1 The CSDMS Software Stack

The CSDMS IF has built the complete CSDMS software stack on several different operating systems including Darwin (Mac), and several flavors of Linux (CentOS, RedHat, and Ubuntu). For each operating system we have created a recipe file that the CSDMS package builder, *bob*, uses to fetch, compile and install the software stack source code.

The CSDMS package builder is now on GitHub:

• <u>https://github.com/csdms/bob</u>

Tasks that will be completed by the end of this funding year will be to construct build files for OS-specific package managers. We will make use of the following native package managers:

- Mac OS X Homebrew (<u>http://brew.sh</u>)
- RedHat and similar (CentOS, Fedora, SUSE, etc.) RPM (http://rpm.org/)
- Ubuntu APT (<u>http://wiki.debian.org/Apt</u>)

# 4.2 The CSDMS Web Modeling Tool (WMT)

The CSDMS Web Modeling Tool (WMT; <u>https://csdms.colorado.edu/wmt</u>) is the web-based successor to the desktop Component Modeling Tool. WMT is a web application that provides an Ajax client-side graphical interface (the **WMT client**) and a RESTful server-side database and API (the **WMT server**) that allows users to build and run coupled Earth system models on a high-performance computing cluster (HPCC) from a web browser.

WMT was designed with four objectives:

- 1. Accessibility. As a web-based application, if you have access to the Internet, you have access to WMT.
- 2. *Integration.* Easily hyperlink from WMT to resources on the CSDMS portal—including model documentation, labs, lectures, tutorials and movies—or to other resources on the Internet.
- 3. *Portability*. WMT has a native JavaScript interface, so it can be accessed on any modern web browser, including tablet and mobile versions of browsers.
- 4. *Maintenance*. Because modern browsers tend to adhere to web standards, which lead to fewer crosscompatibility issues than operating systems, only one version of WMT needs to be developed and maintained.

With WMT, a user can:

- Select a Common Component Architecture (CCA) component model from a list to run in standalone mode;
- Build a coupled model from multiple CCA components organized as nodes of a tree structure;
- View and edit the parameters of the model components;
- Save models to a server, where they can be accessed on any computer connected to the Internet;
- Share saved models with others in the community;
- Run a model by connecting to a remote HPCC where the components are installed.

Although WMT is web-based, the building and configuring of a model can be done offline. Reconnection is necessary only when saving a model and submitting it for a run.

The **WMT client** was designed using the model-view-presenter (or MVP) pattern, which separates the domain logic of an application, where rules are set for how data are stored and modified, from the user interface, where the user interacts with data. This separation of responsibilities makes it easier to test, modify and maintain an application. The WMT client is written with GWT, a toolkit that allows Ajax applications to be developed in Java, thereby enabling the author to employ object-oriented design principles and mature Java development tools such as Ant, Eclipse and JUnit. For deployment on the web, the GWT compiler translates the Java code to optimized and obfuscated JavaScript. GWT emphasizes cross-browser compatibility, and is supported on all modern browsers.

Figure 2 shows an instance of the WMT client running in a web browser, with its primary components highlighted.



Figure 2 Example of the WMT client interface, with primary components highlighted.

The WMT client interface is divided into three panels:

- 1. The *Header panel* provides email and password boxes for a user to sign in to WMT. First-time users are asked to repeat their password for confirmation. Note that the WMT sign is separate from the sign in for the HPCC on which models are run.
- 2. The *Model panel* is where a standalone or a coupled model can be created. To design a model, an instance of a component is chosen at the root of this panel's tree structure. Once included in the tree, the component displays its CCA uses ports as leaves on the tree. By choosing other components that provide ports for these open leaves, a coupled model can be created. A component instance that provides feedback to the coupled model is displayed as a link. The panel also furnishes a set of buttons that allow a user to open, save, and run models.
- 3. The parameters of the model components displayed in the Model panel can be viewed and edited in the *Parameters panel*. Type and range checks are performed immediately on any parameter that is modified.

Information on using the WMT client can be found on the CSDMS portal, including a help document (<u>http://csdms.colorado.edu/wiki/WMT\_help</u>) and a basic tutorial (<u>http://csdms.colorado.edu/wiki/WMT\_tutorial</u>).

The **WMT** server is a RESTful web application that provides a uniform interface through which client applications interact with the CSDMS model-coupling framework. Although opaque to a client, behind the WMT server is a layered system that consists of the following resources:

- A *database server* that contains component, model, and simulation metadata;
- One or more remote *execution servers* on which simulations are launched;
- A *data server* on which simulation output is stored and can be downloaded.

Each of these layers exposes a unique web service API.

The database server provides, as JSON-encoded messages, the component metadata necessary for an end user to couple components, and set input parameters. The metadata includes descriptions of component exchange items, uses and provides ports, as well as user-modifiable input parameters. The database server is intentionally separated from the execution server so that it may be easily and quickly accessed without need to connect to a potentially firewalled or inaccessible execution server.

Execution servers are computational resources that contain the software stack needed to run a coupled or uncoupled model simulation. These servers can range from large high performance computing clusters, to smaller web servers, or even to an end-user's personal computer. The requirements are only that the WMT server has network access to the execution server and that the CSDMS software stack is installed on the server. This includes the CCA-toolchain, the CSDMS framework tools, and compiled shared libraries for each of the component models. Once a simulation completes, its output is packaged and uploaded to a data server where it is stored and from which the end-user is able to download it as a single compressed archive file. The relationship between the WMT client and the WMT server is depicted in Figure 3.



Figure 3 The relationship between the WMT client and the WMT server.

Note that because the WMT server provides an API for each of its layers, other clients—besides the WMT client developed at the CSMDS IF—could be written to access it. Both the WMT client and the WMT server are open source projects, released under the MIT License, with source code available on Github:

- WMT client: <u>https://github.com/csdms/wmt-client</u>
- WMT server: <u>https://github.com/csdms/wmt</u>

We encourage CSDMS members to fork these projects to add their own features, enhancements, and improvements, then create pull requests to merge them back into the original CSDMS projects.

# **4.3 Framework Service Components**

The transition from CMT to WMT highlighted inefficiencies in the CSDMS model-coupling framework, which allowed for refactoring and revisiting of design choices made in the coupling framework. As such much of the CSDMS model-coupling framework was either refactored or redesigned and rewritten. The resulting framework is now leaner, more robust, and significantly more maintainable. The source is now available on GitHub:

- <u>https://github.com/csdms/coupling</u>
- Building and unit testing results through continious integration are available on Travis-CI at: • <u>https://travis-ci.org/csdms/coupling</u>

**Timeline**. The timeline service component orchestrates the timing and execution of a component and its connected service and model components. The timeline component determines the execution time step of a component's uses ports to either a user-requested time step or to a time step based on the time steps of the connected components. In addition, the timeline component is able to cope with 2-way (or circular) couplings. Although not yet implemented, the timeline was written to accommodate future parallelism. In such a scenario, a component's uses ports could, if possible, be executed in parallel with the timeline coordinating the execution and gathering of data.

Time interpolator for grid stacks. The grid stack interpolator service component reads a UGRID formatted grid from a local or remote NetCDF file and provides the data through a BMI to other components. If necessary, the data can also be interpolated in time to provide grids at times that are not provided by the original data file.

# 4.4 Semantic Mediation and Ontologies

CSDMS IF has written a Python package for use with the CSDMS Standard Names. This package will become the Source code for the project is on GitHub: <u>https://github.com/csdms/standard\_names</u>. The standard names package provides tools for working with standard names. With this package users are able to:

- Decompose a standard name into it's constituent parts (object, quantity, quantity operator)
- Compose standard names from constituent parts
- Validate standard names
- Query the standard name database

In addition, the master list of current CSDMS standard names (currently numbering over 900) is also housed on GitHub at: <u>https://github.com/csdms/standard\_names/blob/master/data/master.txt</u>

## 4.5 CSDMS Portal

From June 2013 – June 2014, the CSDMS website averaged 462 page views per day, similar to last reporting year (with 1024 as maximum page views per day, which occurred days after the CSDMS annual meeting). Typically we have 1/3 returning viewers and 2/3 new viewers. The top 3 countries from where the CSDMS website is mostly visited are: United States (39.3%), followed by the UK (5.7%) and China (4.8%), of which the majority used a desktop (93.9%) and only a small percentage used mobile devices (4.1%). The CSDMS website is the first to come up in a Google search, automatically displaying 4 site links, which are the most visited sections of the website (Model download portal, Model portal, annual meeting, and Upcoming events). Site links are shown on privilege by Google (so not controllable in the Google search) and are only shown for nr. 1-search hits, when a page's lifetime exceeds 2 years, and have a Google page rank of at least 2. Sitelinks typically provide more exposure of a website.

Last year, CSDMS became even more active towards its community by: 1) posting CSDMS-related job opportunities (78); reporting upcoming events like symposia, conferences and workshops (56); and tweeting messages to 86 followers on twitter that were CSDMS related (61).

#### Web improvements

a) Web forms (and search queries) are expanded to ensure that CSDMS members can contribute to the CSDMS web without needing any web or wiki knowledge. Through these forms a publication citation database is developed that can be queried such that: a) all publications of a model will be presented, or b) all publications of a CSDMS member will be listed. For the convenience of the web viewer, when populating the DOI field for a publication, a link is automatically generated to the specific journal and visualized at the end of each publication. Publication on a model page will be listed in 3 categories: 1) Overview and general, listing all publications that provide a model overview or a general model description, 2) Applications, listing all publications that show the model application, and 3) Related theory and data, listing publications that expend more upon the applied theory and data behind a model. Publication lists have been automatically integrated to a specific model or set of models or CSDMS member pages, simulation descriptions (See Figure 4). By making the publication database available, we hope to engage our community more, as the service advertises their work. With a small effort, authors expose their work to a larger community. CSDMS-IF has entered 556 model related publication references in the CSDMS publication database.

#### References

Add a publication

#### Overview and general

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- Adcroft, A.J., Hill, C.N., and Marshall, J., 1997. Representation of topograp <u>10.1175/1520-0493(1997)125<2293:ROTBSC>2.0.CO;2</u> (View/edit entry)
- Hill, C, Adcroft, A., Jamous, D., and Marshall, J., 1999. A Strategy for Tera Processors in Meteorology, pages 406-425, World Scientific Publishing Co:l (View/edit entry)
- Hill, C., and Marshall, J., 1995. Application of a Parallel Navier-Stokes Mod Computational Fluid Dynamics: Implementations and Results Using Parallel (View/edit entry)
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- Marshall, J., Adcroft, A., Hill, C., Perelman, L., and Heisey, C., 1997. A fin J. Geophysical Res., 102(C3), 5,753-5,766., <u>10.1029/96JC02775</u>

b) Twitter - web integration. Twitter is a popular social networking site with over a billion registered users and millions of active users every day. Twitter makes it possible to communicate directly with the community, either by sending, forwarding or replying instantly to messages from any computer device. Within the limit of a 140-character tweet, you can post links to the latest paper, meeting, job advertisement or research finding. As part of our effort to involve the community more efficiently, CSDMS started to tweet more actively early 2013. To expose and engage the modeling community to our tweets, we integrated the tweet history on the front page of the CSDMS website (Figure 5). By integrating the tweet history into the CSDMS website it is possible for members to stay informed, even for those that do not follow @CSDSMS. History is archived, so web links can be easy found and visited days after the tweet. Chairs of all the WGs, FRGs, and initiatives are actively approached and involved in providing information that is "tweetable" to the community.

Figure 4 Example of how publications are listed on a specific model page, including a link to the form ("add a publication") to add additional publications.



Figure 5 Snapshot of part of the CSDMS front page, displaying CSDMS tweet history.

c) JSXGraph – web integration. For our model help pages, we want to provide possibilities to other contributors and display functions that are used in models (e.g. differential equations). JSXGraph is a client-based web java application for displaying advanced vector graphics through a web browser. JSXGraph supports several dynamic geometry systems (GeoGebra, Cabri, GeoNext, Cinderella) but can also be used to define a dynamic geometry from scratch in a mediawiki page. JSXGraph is currently integrated as third party extension to the CSDMS web portal. JSXGraph is browser independent, so no additional plug-ins are required, and it uses only minimal bandwidth, making it a fast dynamic mathematics visualization tool. The first function graph examples will be made available before the end of project year 2. Over project year 3, the model help pages as well as the educational labs will be adjusted such that they display the key used functions.

**d)** Newsletters. The Coastal Working Group has started a ~monthly newsletter as part of an initiative to enlarge participation and engagement from its 420 currently registered members. The chair of the Coastal Working Group (Brad Murray) has appointed Chris Thomas (BGS, UK) to lead and coordinate this effort. The newsletters are sent to the Coastal Working Group members through the CSDMS email lists and are also posted as an archive on the Coastal Working Group site (http://csdms.colorado.edu/wiki/Coastal). This is a pilot project to see if newsletters will enlarge the engagement of members of the various WGs, FRGs and Initiatives. If successful, similar newsletters will also introduced for other large WGs, FRGs and Initiatives.

#### Web maintenance

CSDMS cyber infrastructure uses the open software package Mediawiki (http://www.mediawiki.org) and numerous third-party extensions (61 extension as of now) to extend cyber infrastructure capability and to provide the latest cyber tools to web visitors to guarantee the easiest experience to interact through the web. About every year the core software (mediawiki) is significantly upgraded, along with most third party software extensions, to guarantee performance and security and to incorporate new features. It is required by the University of Colorado (CU) to upgrade cyber infrastructure to a newer version when a security upgrade becomes available to reduce possible cyber attacks directed to CU. CSDMS executed the latest major cyber infrastructure upgrade (upgraded to mediawiki v1.21.3, see <a href="http://csdms.colorado.edu/wiki/Special:Version">http://csdms.colorado.edu/wiki/Special:Version</a>) to conform CU standards. Outdated extensions were replaced were needed to guarantee functionality.

#### Website data functionality

CSDMS is in the process of setting up benchmark data collections such that model users can test the strengths and weaknesses of similar models. An experimentalist workshop, organized with help of the EarthCube SEN project, was attended to discuss opportunities to generate a few tank experiment parameter datasets in combination with model input – output datasets that mimic tank experiments. By the end of this project year, we envision to have the first data collections in place to realize this.

Making model data input and output available to the community is as important as providing model source code to the community. This is to 1) be able to see if a model does function once source code is locally downloaded and compiled, and 2) to check if generated model output is similar to suggested output by developer. Different data structures are investigated: a) by integrating test and example data within the source b) by storing the test data separately on a data server. TopoFlow code. and (https://github.com/csdms/topoflow/tree/master/topoflow) now incorporates an example directory and test datasets for most components in the component folder. Storing input/output data with the source has the advantage that models can be tested easily; by downloading the source code you automatically get the datasets. This is also is a disadvantage when you have large test and example datasets. Large datasets will make your model repository large, reducing the download performance. We are in the process of setting up a structure on the CSDMS dataserver to investigate the best ways to set up a structure for test datasets for the various models and model versions in our repositories.

# 4.6 Education and Knowledge Transfer

CSDMS has a defined EKT mission to enable computer model use and development for research in the earth surface processes. CSDMS strives to widen the use of quantitative techniques and numerical models and promote best coding practices. This key objective is met through CSDMS Framework development, making models easier to use through the Web Modeling Tool (addressed elsewhere in this report), and tight integration between the WMT and model theory, metadata, and help pages as an online resource.

CSDMS also aims to enable undergraduate and graduate students (and their instructors) to more easily use models. In 2014 we released the web modeling tool (WMT) (reported on elsewhere in this report), and associated educational material and tutorials. Developed EKT materials are made available through the existing online repository.

# 4.7 Educating Model Users and Developers

CSDMS aims to publish its model codes with extensive documentation to take them beyond black box state. Science practice condemns just manipulating models in terms of their input and then generating output for a user without having knowledge of its internal workings or without being able to get insight in the model engine, or its process routines. It is of crucial importance to know the level of process simplification within a model engine and the implementation into equations and a numerical scheme. Without such transparency the analysis of model output is of much less value. This general mandate is more prominently defined in the CSDMS2.0 phase and a number of support systems are in place or being developed to allow for this transparency.

Any component in the Web Modeling Tool is documented in more detail on the CSDMS wiki (Figure 6 and 7). From within the WMT, a user can easily get to a 1) more extensive model description, 2) notes on the input parameters, 3) key process equations for the model, 4) notes on coupling ports and 5) essential references to the model provided by the original developer or development team.



Figure 6 All components in the WMT have easy live links to online detailed documentation maintained on the CSDMS wiki

? CEM					
					a shoreline due to gradients in breaking-wave-driven alongshore sediment transport. The original CEM has id a wave input module (WAVES).
Extended mo	del introduc	tion			
model was initial coast > 45 degre Although a numb directional wave accurately simula The value in this (2006b) present a Model param CEM does not nee	ly designed to ir es). er of wave (and climate controll ate a specific ge model is in the a more thorough etters ed input files fro	vestigate an instability geometry) parameter: ed by two main input p ographic location in de breadth it offers in rep n description of the mo	y in the s s can be aramete tail but r resenting del parai	shape of the entered, th rs: the asy ather to m g how diffe meters and	bile sediment and its other assumptions are more applicable at shoreline lengths of km's and larger. The a coast caused by waves approaching with 'high' angles (with the angle between deepwater crests and the ne most vital input control for CEM is the wave climate. The current version of the CEM is driven by simplified mmetry of the incoming waves angle and the proportion of high-angle waves. This model is not designed to ore generally represent how a shoreline with highly mobile sediment may respond to varying wave angles. rent wave climates can result in different potentially interesting shoreline configurations. Ashton and Murray theoretical underpinning.
files; as a default	t they are OFF.				
Input Files an	nd directories	Run Parameters	Grid	Output	Grids
Parameter		Description		Unit	
Parameter					
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		ulation time steps ope of the Shoreface	[da [-]		
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Figure 7 A detailed model description associated with the CEM-Coastline Evolution Model

Increasingly, pedagogical research shows the importance of hands-on activities in learning. Students show more learning gains when they work with inquiry-based modules and receive instantaneous feedback (Fogleman et al., 2011). The CSDMS Educational Working Group identified this opportunity for student learning (Campbell et al., 2013), but strategically noted that hands-on modeling labs become more valuable if they are not just about pushing buttons, but instead are combined with mathematical and physics problems based on the careful analysis of the underlying model engine (Schwarz et al., 2009). CSDMS develops an educational repository with modeling labs for graduate and advanced undergraduate students. All of these labs help students run models and analyze output, and highlight some critical aspect of the modeled processes and model engine, the selection of which depend on the learning objective and lesson plan (Figure 7). (http://csdms.colorado.edu/wiki/Labs\_PLUME)

# 4.8 Advanced Modeling Labs for Graduate and Senior Undergraduate Students

CSDMS IF staff designed and improved a series of combined lectures, labs and assignments for a special topics course on 'Surface Process Modeling' in 2013. This material underwent updating to be tightly integrated with the newly released CSDMS WMT in 2014. All components currently available through the WMT have an associated modeling lab posted in the EKT repository (6 labs in total). The course follows a source-to-sink topical progression: from hillslopes to rivers to landscape evolution to coastal processes and eventually marine stratigraphy.

1. Get Started with WMT (the new tutorial)

- 2. River Sediment Supply Modeling with HydroTrend
- 3. Landscape Evolution Modeling with CHILD
- 4. Modeling River Plumes
- 5. River-Delta Interactions with CEM model
- 6. Modeling Stratigraphy in 2-D cross-sections with Sedflux

(7. Final Assignment: designed as an independent modeling study on a unique problem with a relevant model or coupled models as chosen by students, so there is no instructor documentation.)

# 4.9 Science-on-a-Sphere Animations

The CSDMS EKT mission includes a K-12 component as the entry tier to the Quantitative Dynamics Modeling Toolbox. Science On a Sphere (SOS)<sup>®</sup> is a spherical display system approximately 6 feet in diameter which shows "movies" of animated Earth system dynamics, developed by NOAA. There are few earth surface process and modeling datasets in the SOS archive. In 2014, we have developed animations, lesson material and running exhibit 'fact slides' for 3 Science-on-a-Sphere (SOS) animations:

- 1. Global Damming of Rivers, with special focus on the Mississippi Basin
- 2. Global Wave Dynamics (Wave-Watch III)
- 3. Global River Runoff, with special focus on (Water Balance Model-WBM)

The development of the early prototypes of the animations and lesson material has been in close cooperation with the education and outreach team of the Fiske Planetarium at the University of Colorado and NOAA SOS technicians. Fiske Planetarium educators plan to help with a more formal evaluation of impact by doing visitor interviews. Approximately 30,000 people come through the Fiske Planetarium each year. The evaluated lesson material and animations will be made available as datasets through the SOS animation library and becomes available to (ultimately) 33 million people who see Science On a Sphere® every year worldwide. Datasets are scheduled for release in 2014.

# 4.10 Hands-on Clinics and Courses

An important part of CSDMS involves educating our community on disciplinary modeling efforts, and education of code developers by teaching protocols for better transfer of codes, advocating for code transparency, best-coding practices and version control. During the CSDMS annual meeting, which hosted 100+ members in 2014, 10 clinics on models and modeling skills were offered:

Ali Khosronejad	The SAFL Virtual StreamLab (VSL3D): High Resolution Simulation of Turbulent Flow, Sediment Transport, and Morphodynamics in Waterways
Greg Tucker & Daniel Hobley	Creative computing with Landlab: A flexible Python package for rapidly building and exploring 2D surface-dynamics models
Eunseo Choi	SNAC: A 3D parallel explicit finite element code for long-term lithospheric deformation modeling
Courtney Harris	Regional Ocean Modeling System (ROMS)
Chris Jenkins	Carbonate Models Clinic – carbo* suite
Laura Swiler & Adam Stephens	Dakota: A Toolkit for Sensitivity Analysis, Uncertainty Quantification, and Calibration
Mark Piper & Irina Overeem	WMT: The CSDMS Web Modeling Tool
Scott Peckham	Introduction to the Basic Model Interface and CSDMS Standard Names
Monte Lunacek	Interactive Data Analysis with Python
Joshua Watts	Agent-Based Modeling Research: Topics, Tools, and Methods

Post-meeting evaluation shows that the model clinics are one of the highlights of the CSDMS Annual Meeting — well organized and of appropriate length (a few respondents indicated clinics could be longer). Thirty post-meeting evaluation respondents ranked the clinics on average at 4.1 (on a Likert scale 1-5).

# Overeem, I., Piper, M., 2014. WMT: The CSDMS Web Modeling Tool. CSDMS Annual Meeting, Boulder, CO, May 2014. ~30 participants.

Clinic Description: The CSDMS Web Modeling Tool (WMT), the web-based successor to the desktop Component Modeling Tool (CMT, presents a drag-and-drop interface that allows users to build and run coupled surface dynamics models from a web browser on a desktop, laptop or tablet computer (see Section 4.2). The clinic presented an overview of WMT, including an explanation of the user interface, a listing of the currently available models and a discussion of how models can be run in operational mode or in reduced-input mode for teaching. We capped the clinic with a live demonstration of setting up, saving and running a coupled model on the CSDMS supercomputer system.

# Overeem, I. CSDMS WMT software demonstration (15 minutes each for 12 researchers of Chevron, Shell, Saudi-Aramco and Conoco-Phillips), Houston, TX, 7-9th April, 2014.

Demonstration Description: at the Annual Meeting of the American Association of Petroleum Geologists, April 2014, Overeem separately met with representatives of Chevron, Shell, Conoco-Phillips and Saudi-Aramco to present the CSDMS Web Modeling Tool. Demonstrations of the newly released software were limited to around 15 minutes, and demonstrated capability of WMT for stratigraphic modelling purposes. CSDMS 2.0 presentation and short paper were shared with these research teams.

# Overeem, I. CSDMS WMT software demonstration (45 minutes for interdisciplinary team of researchers of DELTAS Project, web-based June 10, 2014. 18 participants.

Demonstration Description: Overeem presented CSDMS modelling framework concepts with a live demonstration of setting up, saving and running a coupled model on the CSDMS supercomputer system. Discussion on specific model architecture for modelling delta processes and data-model connections followed with the interdisciplinary research team and stakeholder representatives.

# Overeem, I., 2014. Modeling of complex landscapes and sedimentary systems: using the CSDMS modelling framework. 2-day clinic at the NCED Summer Institute, University of Minnesota, MN, 19-20<sup>th</sup> of August 2014. ~30 participants.

Clinic Description: The CSDMS Web Modeling Tool (WMT) presents an easy-to-use interface that allows users to build and run coupled surface dynamics models from a web browser on a desktop, laptop or tablet computer. In this hands-on clinic we use a suite of models available through this modeling system, notably HydroTrend, Sedflux and CHILD. The clinic increases efficacy with a high-performance computing system, and quantitative numerical modeling, and addresses in discussions and experiments complexity and predictability of landscape evolution and sedimentary systems.

#### CSDMS Software Carpentry Bootcamp (1 day), Boulder, CO, May 23, 2014. ~40 participants

CSDMS organized a post-annual meeting bootcamp to promote software best practices in our community. A 1-day software carpentry bootcamp was organized as a separate day after the annual meeting and was capped at 40 participants. The bootcamp covered the core computer and programming skills needed to be a productive data analyzer or model user/developer in a small research team:

- the Unix shell (and how to automate repetitive tasks);
- Python (and how to grow a program in a modular, testable way);
- Git and GitHub (and how to track and share work efficiently);

Software Carpentry is a volunteer organization whose goal is to make scientists more productive, and their work more reliable, by teaching them basic computing skills. The Software Carpentry group brought in two experienced instructors especially for this course.

# 5.0 Conferences & Publications

#### 5.1 CSDMS Staff Participation In Conferences & Meetings

May 20	13 to July 2014		
	Water in the Anthropocene	Bonn, Germany	(Syvitski)
07/2013	10th Int'l Conference on Fluvial Sedimentology	Leeds, UK	(Syvitski)
07/2013	IAHS - IAPSO - IASPEI Joint Assembly	Gothenburg, Sweder	n(Syvitski)
08/2013	Stratodynamics—EarthCube Experimentalist	Nagasaki, Japan	(Kettner)
	Workshop		
09/2013	Xiamen University Advisory Committee Meeting	Xiamen, China	(Syvitski)
09/2013	Advisory Committee on Science and Outreach	London, UK	(Syvitski)
	of the CARIAA		
	GSA Annual Meeting	Denver, CO	(CSDMS Staff)
	1st Int'l Workshop on Coastal Subsidence	New Orleans, LA	(Syvitski & Higgins)
	AGU Annual Meeting	San Francisco, CA	(CSDMS Staff)
12/2013	Gilbert Club – Earth & Planetary Science	Berkley, CA	(Kettner)
01/2014	IGBP and IHDP Anthropocene Synthesis	Washington D.C.	(Syvitski)
	Workshop		
01/2014	Meeting of Future Earth Global Environmental	Washington D.C.	(Syvitski)
	Change Projects		
01/2014	Rivers of the Anthropocene	Indianapolis, IN	(Syvitski)
03/2014	EarthCube Stakeholder Assembly Workshop	Washington D.C.	(Syvitski)
03/2014	44th International Arctic Workshop	Boulder, CO	(CSDMS Staff)
03/2014	UNAVCO Science Workshop	Broomfield, CO	(Syvitski)
	AAPG International Meeting	Houston, TX	(Overeem)
	CSDMS Annual Meeting	Boulder, CO	(CSDMS Staff)
05/2014	CSDMS Software Bootcamp	Boulder, CO	(CSDMS Staff)
05/2014		Annapolis, MD	(Syvitski)
06/2014	7th International Congress on Environmental	San Diego, CA	(Syvitski)
	Modelling and Software		
06/2014	1	Greenbelt, MD	(Syvitski)
06/2014	0	Minneapolis, MN	(Syvitski & Xing)
07/2014	7th International Scientific Conference on the	The Hague,	(Syvitski)
	Global Energy and Water Cycle	Netherlands	

# 5.2 Integration Facility Staff Publications — Book Chapters, Journal papers and Newsletters:

#### Submitted/in review July 2013 to July 2014: (IF Staff in bold)

- Allison, M, B Yuill, T Törnqvist, F Amelung, T Dixon, G Erkens, R Stuurman, G Milne, M Steckler, J Syvitski, P Teatini, 2014, Coastal subsidence: global risks and research priorities, EOS Transactions.
- Chen, Y., **Overeem, I., Kettner, A.J.,** Gao, S., and **Syvitski, J.P.M.**, *submitted.* Reconstructing the Flood History of the Yellow River, China: A simulation based on uncertainty and sensitivity analysis. JGR.
- Gao, J., H., Jia, J., Kettner, A.J., Xing, F., Wang, Y. P., Gao, S., *submitted*. The impact of reservoirs on fluvial discharge and sedimentation processes of the Changjiang River, China. Aquatic sciences.

#### Accepted/in press July 2013 to July 2014:

Higgins, S., Overeem, I., Syvitski, J. P. M., Steckler, M., Akhter, S., & Seeber, L., 2014, InSAR Measurements of Compaction and Subsidence in the Ganges-Brahmaputra Delta, Bangladesh, Journal of Geophysical Research.

Syvitski, J.P.M., Cohen, S., Kettner, A.J., and Brakenridge, G.R., *accepted*. How important and Different are Tropical Rivers? – An overview. Geomorphology.

#### Published July 2013 to July 2014:

- Barnhart, K., Anderson, R., **Overeem, I**., Wobus, C., Clow, G., Urban. F. 2014. Modeling erosion of ice-rich permafrost bluffs along the Alaskan Beaufort Sea coast. Journal of Geophysical Research.
- Brakenridge, G.R., Syvitski, JPM, Overeem, I., Higgins, S. A., Kettner, A.J., Stewart-Moore, J.A., Westerhoff, R., 2013. Global Mapping of Storm Surges and the Assessment of Delta Vulnerability, Natural Hazards. 66: 1295-1312.
- Cohen, S., Kettner, A.J., and Syvitski, J.P.M., 2014. Global Suspended Sediment and Water Discharge Dynamics Between 1960-2010: Continental trends and intra-basin sensitivity. *Global and Planetary Change*, 115, 44-58.
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Photo: CSDMS Annual Meeting clinic

# 6.0 CSDMS 2.0: Working Groups & Focus Research Groups

# 6.1 CSDMS Terrestrial Working Group

#### Discussion group findings from 2014 annual meeting

The Terrestrial Working Group met during two breakout sessions at the CSDMS annual meeting in May 2014. The main topics addressed during these sessions were (1) overview of group activities and community-funded CSDMS projects, (2) potential models for wrapping with a basic model interface (BMI) for compatibility/interoperability with the Web Modeling Tool (WMT), and (3) model intercomparison. In addition, a third "mixed group" breakout session was convened on the topic of uncertainty quantification; results pertinent to the Terrestrial group are reported here.

#### Priorities for model inclusion in CSMDS model repository and WMT

The Terrestrial and Geodynamics groups called for incorporation of at least one 3D crustal deformation model, which could then be coupled with a surface processes model to study the dynamic interactions among tectonics, climate, lithology, and topography. One candidate is SNAC, written by Prof. Eunseo Choi of the University of Memphis. SNAC is a 3D thermo-mechanical model that addresses large-scale deformation in settings with complex rheology. Prof. Choi has obtained funding to study the interaction between tectonics and erosion using coupled modeling, and is working with CSDMS staff to develop a BMI for SNAC. He will couple SNAC with the landscape evolution model CHILD, with assistance from CHILD team members Greg Tucker and Nicole Gasparini as needed.

The Terrestrial and Geodynamics groups also plan to further study the possibility of working with Underworld, a code developed at Monash University by Louis Moresi and colleagues. Prof. Moresi presented Underworld to the CSDMS community during a keynote lecture at the 2013 meeting. Underworld is a "3D-parallel geodynamic modelling framework capable of deriving viscous / viscoplastic thermal, chemical and thermochemical models consistent with tectonic processes, such as mantle convection and lithospheric deformation over long time scales." The code differs from SNAC in that it uses a Lagrangian particle-in-cell finite-element numerical method. Underworld has been applied to a wide-ranging set of solid-earth phenomena (https://www.underworldproject.org/models.html).

The Terrestrial group is also interested in obtaining a wrapped model for 2D glacier dynamics. Although such a model (GC2D) already exists in the CSDMS repository, there is a need for a fairly simple glacier-modeling program that interfaces easily with data and can be quickly deployed to study various topics in ice dynamics and its coupling with hydrology, landscape evolution, and lithosphere flexure. Andrew Wickert of the University of Colorado has recently developed a Python-based glacier dynamics model (written using the Landlab platform, which is described below). The code is already close to full CSDMS compatibility. The group recommends that this code be fully wrapped as a component in WMT. We note that the code interfaces with the open-source GIS program GRASS.

The Terrestrial group noted a need for a good model of sediment flux and topographic change resulting from mass wasting processes such as landslides, rockfall, debris flows, and similar gravitational movements. However, although engineering models exist to describe slope stability, the development of models that predict the long-term evolution of topography under such processes is still in its infancy. One model to consider is a 2D earth-flow model recently developed by Prof. Adam Booth of Portland State University (Booth et al., 2013).

The Hydrology Focus Group discussed the need for BMI-wrapped models of catchment rainfall-runoff and land-surface hydrodynamics. These would be of benefit to the Terrestrial Group for exploring coupling between hydrology, sediment transport, morphodynamics, and landscape evolution.

The group noted that many potentially useful models are available as modules in GRASS GIS. The group recommends that the CSDMS integration facility team explore the potential for a standard interface to GRASS modules. If it were possible to create such an interface without the need to directly modify the modules themselves, this would immediately bring a whole host of components into the CSDMS WMT fold.

Finally, the group discussed the need for incorporating a package for parameter optimization and uncertainty analysis. The need for automated parameter optimization is likely to continue to grow in the earth-surface dynamics community, as a means of testing models against increasingly sophisticated data sets (such as those from lidar surveys) and a means of comparing and testing alternative models. Likewise, the need for uncertainty analysis is growing (as the theme of the 2014 meeting attests). Four packages to consider are PEST, Ostrich, UCODE, and Dakota.

#### Model intercomparison

The group noted that two areas for fruitful model intercomparison are fluvial morphodynamics and landscape evolution. Different types of model intercomparison address different issues: (1) differences in numerical implementation of the same governing equations, (2) different mathematical representations of the same processes, and (3) different processes. Simple comparison between codes can highlight differences in all three issues, and thereby highlight both strengths and weaknesses in numerical solution schemes, and differences in the predictions of alternative formulations that could be tested against data.

The group discussed experimental data sets as bases for model testing and intercomparison. There was debate as to the value of such comparisons. On the one hand, experiments in morphodynamics and landform evolution are imperfect representations because of scale issues (related, for example, to viscous length scales). On the other hand, if a model cannot reproduce the highly controlled environment of a laboratory, its applicability to field cases might be called into question. Dialogue between model developers and experimentalists are needed.

The group also expressed a need for "natural experiment" data sets that capture the evolution of a terrestrial landscape or "morphoscape" with enough quantitative control on initial and boundary conditions and system evolution to provide a rigorous test (Tucker, 2009). Potential cases include: cinder cones, small deltas, agriculture experimental sites (e.g., Walnut Gulch), cosmogenically dated catchment-fan systems, critical-zone observatories, large floods with "before and after" lidar, dam removals and/or breaches, published tectonic geomorphology case studies, badlands, and marine terraces. There is also a need to develop a standard set of test metrics and test cases for landscape evolution models.

#### Uncertainty quantification

Parameter optimization and uncertainty quantification have great potential across the various disciplines of earth-surface dynamics. This community is generally not as well versed in these topics, for example, the groundwater hydrology community. Therefore, there is a need for training in basic principles and applications of uncertainty analysis.

#### Working group activities and funded CSDMS projects in the community

#### Thematic discussion groups

During the past year, two thematic discussion groups were formed. One group, led by Francis Rengers (University of Colorado), is focused on wildfire and its impacts on erosion. A second, led by Arnaud Temme, focuses on modeling soil development and soil erosion. Both groups are in a stage of informal (mostly email-based) discussion. Both group leaders have expressed an interest in using Landlab to develop models related to these topics.

#### Landlab project

Recently, a group of CSDMS members led by Greg Tucker obtained funding to develop a Python-based software framework, called Landlab, to support rapid numerical model development and coupling. The

seven-member team presented a clinic on Landlab at the 2014 meeting. Landlab is intended to make the process of creating models and components easier by providing an underlying "gridding engine" to create and manage 2D grids and associated data, and by providing other capabilities such as standardized I/O. The choice of Python is based on the community's current embrace of high-level, interpreted, function-rich commercial packages that provide automated array operations.

The software is also intended to facilitate componentization by providing a "built in" BMI with each Landlab component. Wickert's glacier dynamics model, noted earlier, provides an early proof-of-concept. The team recently applied for a second round of funding, which if provided would support expanded community outreach and training, increased performance (through embedded C functions), new components, and other functionality. Landlab is seen as a natural extension to the CMT/WMT because it provides support for development and coupling of new components, and because components that are coupled within a Landlab model share grids and data among themselves, thereby eliminating the overhead of translating between multiple grids and data structures.

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# 6.2 Coastal Working Group

New Appointments: Two new Vice Chairs have been appointed within the Coastal Working Group:

- Hans-Peter Plag (Old Dominion Univ.) will lead the Coastal Vulnerability Initiative (CVI), bringing his experience leading organizations addressing aspects of coastal vulnerability. Initial plans include writing a white paper (for submission to a journal), building on the results of the initial discussion at the CSDMS Annual Meeting in 2013.
- Chris Thomas (British Geological Survey) will lead on community engagement, to widen communication and information exchange within the community. Initial plans include the monthly circulation of an interactive Working Group newsletter, in which working group members can share with each other scientific and funding successes, job and assistantship opportunities, etc.
- Announcements of liaisons between the Working Group and CVI and other organizations/communities will come soon.

#### Model Prioritization/Progress on Model BMIs

As part of the new CSDMS Strategic Plan, each Group is tasked with wrapping (at least) one model per year with a Basic Model Interface (BMI)—i.e. the 'Roadmap'

- Each choice requires community demand and a champion
- Progress (priorities identified in CSDMS Strategic Plan):
  - SWAN: BMI underway (success this year likely)
  - o Rocky Coastline Evolution Model (RoCEM): BMI underway (success this year likely)
  - o Dynamic river avulsion Component: development, BMI planned (success next year likely)
  - Hydrodynamic model capable of storm surge simulation
    - Identified as priority
    - Not linked to compelling science question or funded project; Champion needed
    - May require spurring collaboration to address a question requiring coupling

• Delft3D is a possibility (BMI being considered)

**Model Intercomparison Plans:** Please see the results of the joint Coastal, Marine, and Carbonate Groups discussion from the Annual Meeting in section 6.3.

# 6.3 Marine Working Group

A series of short-term (1-2 yr) objectives are outlined in the CSDMS Strategic Plan, including:

- Developing a set of models that can be coupled via BMI.
  - Toward this, SWAN is being wrapped as a BMI, and Delft-3D is being considered (both as mentioned in the Coastal Working Group notes).
  - Marine working group called for an atmospheric / wind model. Scott Peckham is working with others to incorporate WRF by wrapping it within a BMI.
- Developing a "simplified" or "easier to use" hydrodynamic model to incorporate in the CSDMS toolbox. Toward this an idealized continental shelf model was presented as a CSDMS clinic. The model uses ROMS (the Regional Ocean Modeling System) to solve for hydrodynamics, salinity, and sediment transport fields for a planar-shaped continental shelf onto which a freshwater plume flows. The ROMS model has been ported to the CSDMS computer, beach, and we are calling this implementation "riverplume2", or "ROMS-LITE".
- Incorporating (wrapping in a BMI) a finite-element model (needs a champion)

#### Model inter-comparison projects (MIPS): Discussion at Annual Meeting (with Coastal and Marine Working Groups, and representation from Carbonate and Chesapeake Focused Research Groups)

The Chesapeake Research Focus Group, affiliated with both the Coastal and the Marine Working Groups, made substantial progress towards model inter-comparison through the Coastal Ocean Modeling Testbed project:

- A model intercomparison project funded by NOAA, with a requirement to advance operational models; this project is winding down and producing final reports and peer-reviewed publications.
- The overall focus of the project has been on three types of modeling efforts: ecosystem models that estimate oceanographic productivity (chlorophyll, oxygen dynamics); storm surge operational models; and water quality in Chesapeake Bay and Gulf of Mexico. The Chesapeake Focus Research Group was involved in the Chesapeake Bay portion of the testbed.
- Compared 5 models: Army Corps model for Chesapeake, and 4 versions of ROMS that used the same hydrodynamic equations, but had different resolutions, boundary conditions, O<sub>2</sub> dynamics and water quality, and different model inputs.
- Results and Contributions:
  - Studies within the project have explored the use of various skill metrics. When comparing models, it is valuable to consider concise quantifications of model skill. Useful skill metrics evaluated the mean and variability of model estimates compared to the data, and compared to seasonal trends in the data.
  - Different models have different skill(s) and can fill different roles in scientific inquiry. For example, a model using a very simple, empirically-based formulation for oxygen dynamics may have as high a "skill" as a more complex, process-based model. But, the simpler model would be of little use for applications beyond the conditions within which its empirical relationships were derived.

- The differences that were seen model skills for distinct implementations of the same model could be as significant as those for an implementation of a completely different model. Just testing the parent models, i.e. ROMS compared to another hydrodynamic model, isn't necessarily the relevant question because different implementations of ROMS could have very different skill scores.
- Several publications have been produced from members of the Chesapeake Focus Research Group. For examples, see:
   Luettich, R.A., et al. "Introduction to special section on The US IOOS Coastal and Ocean Modeling Testbed." *Journal of Geophysical Research: Oceans* 118.12 (2013): 6319-6328.
   Bever, Aaron J., et al. "Combining observations and numerical model results to improve estimates of hypoxic volume within the Chesapeake Bay, USA." *Journal of Geophysical Research: Oceans* 118.10 (2013): 4924-4944. And

#### Shallow Tidal Environments:

Initial approach: Provide generalized conditions (SSC, Tidal Range, etc.) based on 2 or 3 well studied locations (e.g. Mississippi Birdfoot diversions, Venice Lagoon, North Inlet...); Elicit modelers using a diversity of models approaches to address common questions:

- A) For a vegetated surface at elevation X (below high tide level), what will the accretion rate be?
- B) What information does your model need to determine that?
- C) What types of models could provide that needed information?
- D) And also A) C) for an unvegetated surface at elevation Y

This approach will both **illuminate the commonalities or divergences** of results in a wide range of models (from 0-dimensional to hydrodynamic-explicit), and **clarify useful sets of model couplings** Shelf/Estuaries

- 1. For model data intercomparison, the marine groups encourage that we seek out morphodynamic data sets. The technology is advancing rapidly in that framework.
- For model model intercomparison it may be worth approaching ONR to see if they would be interested in having models developed as part of recent DRIs be part of an intercomparison study. These studies have both excellent data sets and a variety of models implemented, but to date, funding has not been provided for intercomparison.

# 6.4 Cyberinformatics and Numerics Working Group

The Cyberinformatics and Numerics Working Group has now reached a membership of 172. At the 2014 CSDMS Annual Meeting in Boulder, the WG had useful discussions during the breakout sessions, which resulted in the following two initiatives:

1) Several WG members noticed that a large number of problems of interest to CSDMS members in all groups involve, in one form or another, the tracking of interfaces. This applies, for example, to the evolution of a coastline, the advancing or receding boundaries of a glacier or ice sheet, or the surface of a sediment bed on the seafloor. Frequently, current simulation approaches for such interface tracking problems employ very low-order, coarse numerical methods that may substantially reduce the accuracy of the underlying simulation model. On the other hand, the scientific computing community in recent years has developed a novel class of numerical approaches that allows for much higher fidelity interface tracking algorithms. This approach is generally known under the broad terminology of 'level set methods' (S. Osher and R. Fedkiw 2002 Level Set Methods and Dynamic Implicit Surfaces, Springer Verlag). This approach has become quite mature in recent years, so that it may offer substantial advantages in the modeling of many problems of interest to the CSDMS community. Hence it was suggested that for the 2015 CSDMS Annual Meeting, we should invite a speaker

from the scientific computing community who could provide a broad introduction, and perhaps a clinic, on level set methods.

2) Vice-chair Scott Peckham and Chair Eckart Meiburg have initiated the compilation of a repository of solutions to single- and multi-phase flow problems that can serve as validation cases for computational codes. This solution repository contains four different types of solutions: (i) Exact solutions of the potential, Stokes or Navier-Stokes equations; (ii) Similarity solutions that typically require a coordinate transformation so that they can be compared to numerical solutions; (iii) Asymptotic solutions that are valid in some limit where a certain dimensionless parameter (such as the Reynolds number) becomes very large or very small; (iv) Benchmark computational solutions, i.e., well-established numerical solutions that have been confirmed so many times that they can serve as benchmark data for testing new computational codes. Having a repository of such model solutions readily available to the CSDMS community should facility the validation process for computational models, and result in significant time saving for model developers.

Several of the invited keynote presentations and clinics at the 2014 CSDMS Annual Meeting had a strong numerical/computational component. For example, Jim McElwaine of Durham University (UK) gave an outstanding keynote talk on "Modeling Granular Flows," which discussed computational, experimental and scaling issues of granular flows. Tom Hsu (University of Delaware) gave an excellent keynote talk that discussed physical insights gained on "Wave-driven Fine Sediment Transport through 3D Turbulence Resolving Simulations." Ali Khosronejad of St. Anthony Falls Lab at the University of Minnesota discussed advances in our understanding of river flows as a result of highly resolved large-eddy simulations, and he provided a clinic that focused specifically on the SAFL Virtual StreamLab modeling tool.

# 6.5 Education and Knowledge Transfer Working Group

The CSDMS EKT Working Group strives to develop and transfer CSDMS tools and knowledge to the following groups:

- •Researchers with model and visualization tools
- •Planners with decision-making tools to run scenarios
- •Educators with pre-packaged models

For our educational materials, we strive to provide materials that help develop quantitative skills, and critical evaluation of model assumptions and outputs. Our principal education audiences are university students, professionals, teachers at the secondary school and college levels, and the general public. To document our progress, we provide below a description of our short and longer-term goals, and our progress towards those goals.

#### Short-term action plan to achieve long-term goals — Goals over 2013-2016:

#### **CSDMS** Course Materials

Call to CSDMS community for contribution of exercises and assignments with modeling focus at a range of educational levels, with goal of at least one contribution per group WG.

- Polish and post products
- Develop simple assessment rubrics
- Distribute to pilot team of at least one person per WG for classroom use, with assessment
- Compile results and experiences and prepare/submit paper to Journal of College Science Teaching, with plan authors and testers as co-authors
- Hold a clinic at CSDMS Annual Meeting: "Bringing CSDMS to the classroom".
- Promote development of web-enabled CMT environment, to circumvent complications of getting large groups to use HPC
- Consider posting to Carleton College Earth Science Education website

- Implement high quality visualization for all products
- consider uncertainty for all products

Promote development of web-enabled CMT environment, to circumvent complications of getting large groups to use HPC

#### Education and research for non-specialists

Develop a streamlined model packages for classroom and researcher use, as binaries or simple CMT implementations

- Query CSDMS community to identify target models
- Componentize and/or prepare stable executables for offline use
- Prepare test cases submitted by user groups or developers
- Promote development of web-enabled CMT environment, to circumvent complications of getting large groups to use HPC
- Implement high quality visulalization for all products
- Consider uncertainty for all products
- Consider developing test cases for existing componentized models for educational use and tutorials for non-specialists, one or more per WG

#### Year Two and farther out: Coupling between GIS and CMT

- Seek out and advertise the existing proof-of-concept examples
- Develop tool to couple GRASS GIS and CMT
- Query end-users to identify key modeling tools and GIS environments for future implementation
- Promote development of web-enabled CMT environment, to circumvent complications of getting large groups to use HPC

#### **Progress Toward Goals**

WMT Release and WMT Teaching Modules. Development of a web-based supercomputing interface was identified in 2013 as an important need of the EKT community. The CSDMS Web Modeling Tool (WMT) was released during the 2014 CSDMS Meeting, and is a major step forward in streamlining educational use of CSDMS HPC models. New WMT teaching modules developed by I. Overeem include:

- "Getting Started with the WMT;"
- "Sediment Supply to Global Oceans" (a WMT module using WMT-based Hydrotrend and spreadsheet models to explore effects of climate change on riverine fluxes);
- "Plume Modeling with the WMT," which uses the PLUME model to explore hypopycnal plume dynamics;

These teaching modules augment existing modules at: http://csdms.colorado.edu/wiki/Labs\_portal

ROMS LITE is a simplified version of the Regional Ocean Modeling System and was introduced by C. Harris at the CSDMS Annual Meeting. Development of ROMS LITE was identified in 2013 as an important step towards making complex grid-based models more accessible for educational use. Our goal for the present year will be to componentize ROMS LITE to allow use in the WMT environment.

Science on a Sphere (SS, <u>http://sos.noaa.gov/What\_is\_SOS/index.html</u>) is a NOAA global modeling outreach project. Contribution of global model simulations to SOS was identified as a short to medium term EKT goal in 2013. CSDMS EKT is working with NOAA scientists to bring simulations online in Fall 2014 in the following topical areas: hydrology, ocean waves, and human impacts. Our goal for the upcoming year will be to query CSDMS members and others for additional global simulations that can be added to SOS.

Continued Modeling Support for NCED. CSDMS will continue to provide clinics at the National Center for Earth-Surface Dynamics (NCED) summer institute.

Development of Stand-Alone CSDMS Model Labs. CSDMS EKT participants have developed teaching labs for the Kim et al. (2009) delta-progradation model and SEDTRANS05 (Neumeier et al., 2008) that can be run on local computers effectively without supercomputer access.

During the upcoming year, EKT goals specific to the above items will include deployment of these WMT and stand-alone teaching modules to multiple university classrooms, along with assessment rubrics, to develop teaching experiences and educational data that will contribute to a short educational methods journal paper. We will also solicit contributions from other working groups for lab development and testing. We will also continue working towards our other objectives, identified above.

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# 6.6 Carbonate Focus Research Group

Recent & current C-FRG activity includes:

- Development and sharing of the Carbo\* organism knowledge base. This is an Excel based compilation of quantitative data on the growth rate, life habits and associated sediment accumulation rates for a range of modern carbonate-producing fauna. Current content is mostly modern corals, but the data format is very flexible and compatible with both modern and ancient fauna. A prototype version of the OKB is available at <a href="http://csdms.colorado.edu/wiki/Life\_Forms\_data">http://csdms.colorado.edu/wiki/Life\_Forms\_data</a>
- Development of carbonate forward models under the C-FRG Carbo\* framework is taking place in University of Colorado, Boulder, Royal Holloway University of London, and NOVA Southeastern University, Florida.
- C-FRG were present at the May 2014 CSDMS meeting where a carbonate modelling clinic had some lively discussion of carbonate modelling at different scales, including with models from the Carbo\* collection.



Figure 8 Output from CarboCAT run showing carbonate strata deposited in a synrift setting

• Initial work has started to create a carbonate scenario for use with ROMS\_lite. The plan is to use a carbonate model to define bathymetry as input for flow modelling in ROMS\_Lite

#### Plans for the future:

- The C-FRG maintains the intention to produce a componentized version of one of the Carbo\* models
- Consider interaction with other models in CSDMS e.g., X-Beach, or oyster bank predictions for other shallow marine and estuarine models
- Recent work in the group suggests efforts could be refocused into modelling more biological and less stratigraphic processes. This possibility requires further investigation, for example to identify collaborators from the Life Sciences to work with, and define a plan of work that could feed into other elements of CSDMS

# 6.7 CSDMS Hydrology Focus Research Group Breakout Sessions

#### **Updates on Working Group Activities**

The CSDMS Hydrology Focus Research Group is co-sponsored with the Consortium of Universities for the Advancement of Hydrologic Science, Inc. (CUAHSI). At last year's CSDMS annual meeting, Hydrology FRG members discussed short, medium, and long-term goals that we seek to achieve through our working group activities. These goals are listed on pages 26-27 of the 2013 CSDMS Strategic Plan.

The first short-term goal was to "Establish ways of collaborating between related activities that are currently happening within the hydrology community." We have done this through our group's membership in NSF projects such as the CUAHSI HydroShare project and NSF EarthCube projects. A common theme across these projects is model metadata and semantics, which if done in a standard way, will provide interoperability across systems like CSDMS and HydroShare. Scott Peckham is a key member in this activity as PI of an Earth Cube award and has presented to the HydroShare group his work on the CSDMS Standard Names. These names will be important to the HydroShare project in its efforts to create metadata for hydrologic resources (data and models) that groups or individuals wish to share with others.

The second short-term goal was to "Identify mechanisms for having more hydrologists participate in CSDMS." The Hydrology FRG membership grew to 410 members adding 34 members since writing the Strategic Plan report. We are one of the largest groups in CSDMS. Many of our models are being modified to be compatible with the CSDMS Basic Modeling Interface (BMI) standard so that they can be used within the Web Modeling Tool (WMT). We continue to advertise the Hydrology FRG and CSDMS in general at conferences attended by hydrologists with interests in modeling and software tools. For example, we had a strong presence at the International Environmental Modelling & Software Society (iEMSs) conference in June including a keynote address by James Syvitski, an invited talk on the CSDMS Standard Names by Scott Peckham, and an invited talk on the CSDMS Hydrology FRG by Jon Goodall.

The third short-term goal was to "Propose a session on 'Community Tools for Advancing Hydrologic Science' at the American Geophysical Union Fall Meeting." This was done in collaboration with CUAHSI and resulted in a successful session that included 17 presentations. We also had a session on a similar topic at the iEMSs meeting in an effort to continue to grow the community of researchers focusing on designing, building, and applying community tools to advance hydrologic science.

#### Discussion of Group Findings from the Annual Meeting

The major focus of Hydrology Focus Research Group breakout discussions at the 2014 Annual Meeting was on model intercomparison. In hydrology, there have been many past examples of model intercomparison efforts in recent decades. One example was the Project for Intercomparison of Land surface Parameterization Schemes (PILPS). The topic of model intercomparison also continues to be a popular topic within the community (e.g., Doherty and Christensen, 2011; Foglia et al., 2009; Maxwell et al., 2014).

A clear consensus among the group was that performing thorough and comprehensive model intercomparisons for hydrologic models, and moreover for hydrologic models coupled to other earth dynamics models, remains a significant research challenge. Hydrology models vary across scales from hillslopes, to catchments, to regional models, to global models. Within each class, different process representations are resolved so comparisons of hydrologic models across these scale-based classifications may not be possible. Also, different datasets become critical at different spatial scales. The reliance on publically available data for catchment, regional, and global scale models makes data collection, synthesis, and management a high priority in order to obtain accurate models.

Despite these challenges, there are general characteristics common to all hydrologic models that could form the basis for cross-scale comparisons. These include what input and output data are associated with the model, the method for land surface discretization (i.e., mesh generation), the data source for parameterization of the model and for forcing the model, etc.. A possible role for the CSDSM Hydrology FRG could be to work to develop this list of model characteristics that would support model intercomparison. The result would be a taxonomy extending the taxonomy of catchment-scale hydrologic models put forth by Kampf and Burges (2007) that could be used to classify the 53 hydrologic models currently indexed within the CSDMS model repository.

#### Plans for the Future

Given the interest within the group in model intercomparison, a focus for the group over the coming year should be to improve the means for classifying and comparing models based on general characteristics of the models. The CSDMS team has begun this activity by collecting model metadata for each model inventoried within the CSDMS model repository. Extensive model metadata that is standardized and machine-readable could provide an opportunity to automate model intercomparisons that focus on the inputs, outputs, process representations, numeric, and other characteristics of the models within CSDMS. This is a different type of model intercomparison than what has been done in the past where the focus is not on comparing the output generated by a set of models for specific modeling case studies, but rather trying to capture the properties of the models, including their inner structure, in a general way that would allow for intercomparison of model long term goals expressed in the 2013 CSDMS Strategic Plan of "Establishing methods for model benchmarking and tests to asses model skill" and "Making hydrologic models more open and transparent for both scientific investigations and to support policy and decision makers." It would also complement efforts in the CUAHSI community to create the Hydroshare system that includes the goal of sharing hydrologic models contributed with standardized model metadata.

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# 6.8 Chesapeake Focus Research Group

The Chesapeake Focus Research Group (FRG) is a partnership between CSDMS and the Chesapeake Community Modeling Program (CCMP, <u>http://ches.communitymodeling.org/</u>), which is currently run by the Chesapeake Research Consortium (CRC). CCMP developed as the Chesapeake Bay research community came together with the common goal of cooperatively building an open source system of watershed and estuary models. Through support from CRC member institutions and the NOAA Chesapeake Bay Office, CCMP modelers have committed to developing a modeling framework that will enable free and open access to code specific to the Chesapeake Bay region. Together, CCMP and the Chesapeake FRG are striving to develop a comprehensive model system consisting of interchangeable individual modules covering diverse aspects of hydrodynamics, ecosystem dynamics, trophic exchanges, and watershed interactions.

#### Chesapeake FRG Progress August 2013 to July 2014

- Chesapeake FRG/CCMP activities over the past year centered on planning and hosting the 2014 Chesapeake Modeling Symposium (CheMS'14) held in Annapolis, MD, on May 28-29, 2014 – see <u>http://www.chesapeakemeetings.com/CheMS2014/</u>. Example CSDMS-relevant aspects of CheMS'14 included the following:
- A plenary keynote presentation at CheMS'14 was given by CSDMS Director James Syvitski.
- Members of the CheMS'14 Planning Committee included the Chair of the CSMDS Chesapeake FRG, the Chair of the CSDMS Marine Working Group, and the Chair of the CSDMS Critical Zone FRG. Also, an additional 16 CSDMS members attended the conference.
- Special sessions at CheMS'14 focused on many CSDMS-relevant topics, including "Successes and Strategies for Model Coupling for Chesapeake Bay and related Systems", chaired by CSDMS member Courtney Harris, and "Unstructured Grid Modeling of Estuaries and Coastal Waters", chaired by CSDMS member Wen Long.

#### Chesapeake FRG Short-Term Term Goals

- Continue to populate the CSDMS with existing open-source Chesapeake Bay region models.
- Pursue avenues for group proposals including funding for full-time or nearly full-time Chesapeake FRG, such as a dedicated post-doc.
- Give priority to Chesapeake FRG related projects which focus on models with management implications, such as land use, water quality, ecosystem function, storm surge, etc.

#### Chesapeake FRG Intermediate Goals

- Train members of the Chesapeake FRG on use of CSDMS tools.
- Construct very simple land use and water quality box models for a Chesapeake FRG "sandbox" for members of the Chesapeake FRG to practice linking and implementing models within CSDMS.
- Post key common forcing data sets at CSDMS.

#### Chesapeake FRG Long-Term Goals

- Implement additional distinct, swappable land use models, hydrodynamic models, water quality models, ecosystem models, etc., in BMI format at CSDMS.
- Utilize CSDMS to make side-by-side comparisons of model performance and differences in output by systematically swapping model components.
- Utilize CSDMS to perform ensemble modeling (i.e., using multiple distinct models) of future Chesapeake environmental conditions under various management scenarios.
## 6.9 Geodynamics Focus Research Group

The Geodynamics FRG had an excellent inaugural year! At its inception in early 2013, the Geodynamics FRG set several immediate goals, including reaching out to the geodynamics community through GeoPRISMS and CIG (Computational Infrastructure for Geodynamics) and seeking feedback from the community on our overall strategy for moving forward. To facilitate this process, co-chairs Upton and Behn convened (with John Jaeger) a special session at the 2013 Fall AGU meeting. The sessions EP33D and EP43E44A "Exploring the interplay between solid Earth tectonics and surface processes from mountains to the sea" had 44 submitted abstracts and both the poster and oral sessions were very well attended. We also organised a GeoPRISMS mini-workshop "Exploring the interplay between Solid Earth Tectonics and Surface Processes using Community Codes":

http://www.geoprisms.org/mini-workshops/32-agu/miniworkshops/452-csdms-mini-workshop-agu2013.html

The workshop, held Wednesday evening of AGU week, had ~30 scientists in attendance with a wide range of interests spanning field-based to modeling studies, attended the workshop. Together with the AGU sessions, the mini-workshop created an opportunity to bring together members of the long-term tectonics community with members of the CSDMS community, particularly those interested in surface processes in actively deforming terrestrial settings. The workshop began with informal discussions over snacks and posters. The formal part of the evening began with a welcome and introduction from Peter van Keken, the incoming chair of GeoPRISMS. Phaedra Upton, co-chair of the Geodynamics FRG introduced CSDMS and the Geodynamics FRG. She was followed by Irina Overeem (CSDMS) who gave an overview of the support, website, modeling tool and educational repository offered by CSDMS. Three invited speakers, Ritski Huismans, Brian Yanites, and Louis Moresi then shared their thoughts and experiences using coupled modeling approaches to link solid Earth tectonics and surface processes with such different spatial and temporal scales.

Following these three presentations, the floor was open for discussion. Themes that arose included:

- The potential for more collaboration between CSDMS and the long-term-tectonics working group Computational Infrastructure for Geodynamics (CIG).
- The importance of coupling as a research direction given the potential for feedbacks between surface processes (e.g., erosion and re-deposition) on long-term tectonic processes. However, this coupling needs to be handled properly, and this requires including researchers from both communities. In particular, the mismatch of spatial and temporal scales between tectonic and surface processes is a major computational challenge. Significant discussion focused on the best computational methods to deal with these different scales. As the community, we need to think about whether we should be moving toward meshless methods.
- The importance of bookkeeping for stratigraphy. In coupling between a landscape evolution model and a tectonic code, the overlap is not just the 2D land surface, thus coupling needs to be in 3D and extending to a depth beneath the earth surface that record deposition.
- One action item that came out of the meeting is that there is immediate value in coupling a highresolution 2.5D tectonic model with a landscape evolution model. Specifically, while 3D is essential for some problems it is not necessary for all problems, and often a 2D model output (extrapolated into the 3<sup>rd</sup> dimension) is sufficient and has the advantage of being higher resolution and faster to run. Therefore, it was proposed that the Geodynamics Focused Research group work to release a 2D model into CSDMS soon. This model could be coupled with existing landscape evolution models to produce some simple test cases to look at key feedbacks between fault evolution and surface processes.

These initial discussions on coupling surface processes with long-term tectonics models were continued at the annual CSDMS meeting. Peter Koons gave a keynote presentation at the workshop on the Failure Earth Response Model (FERM), a new framework to unify the physical description of landscape dynamics between the surface domain of geomorphic processes and the tectonic domain of Earth deformation. Eunseo Choi gave a clinic on SNAC, a 3-D FLAC based code for geodynamics. In addition, the poster sessions at the annual meeting provided an opportunity for researchers and graduate students to present recent research results. At least 3 different numerical approaches were presented for coupling surface processes with long-term tectonic modeling and these fostered discussion between the various groups.

The annual meeting also provided time for continuing the discussions on future directions that were initiated at the AGU GeoPRISMS mini-workshop. Specifically, a plan was developed to move forward with the development and release of several coupled models. Choi has funding to wrap SNAC for the CSDMS Web Modeling Tool and plans to complete this over summer 2014. In addition, there was support for wrapping Underworld as an additional 3-D long-term tectonics code in the CSDMS WMT. We have contacted Underworld developer Louis Moresi and plans are being developed for Underworld developers to work with CSDMS to achieve this goal. Beyond these specific codes, there was also discussion for future development of meshless methods and coupling of long-term tectonics codes with ice-sheet models.

## 6.10 Anthropocene Focus Research Group Meeting

People present: Kathleen Galvin, Isaac Ullah, Kimberly Rogers, Joshua Watts, Irina Overeem, Atilia Lazaar, Alexy Voinov

## 1. Action Items:

- The group suggested an AGU 'invited' (perhaps IGBP sponsored) session be organized on "Modeling the Anthropocene" or 'Earth Systems and Human Dimensions Modeling' or 'Modeling Social Processes with Earth System Dynamics' for the December 2015 meeting. Isaac Ullah and Kimberly Rogers have agreed to help organize a session.
- Does CSDMS have the tools in place to support human-environment research? What does it need to be an incubator of research and proposal writing? (e.g., GRASS, Python) Need input on this.
- Is 'Anthropocene' a useful term for this group? Some argued that people have had a large impact on earth system processes much earlier than is currently thought (e.g., since the Neolithic rather than the Industrial Revolution). Others said that the Anthropocene occurred with the human impact signal became global. It was discussed that 'Human Dimensions' might be a more useful term for this group. HDFRG.
- Create a modular library in the CSDMS: models in the repository could be "tagged" by time step, appropriate spatial scale to enable identification of suitable models for coupling
- Encourage learning/use of Python as 'universal language' for models intended for coupling
- 'Conceptual coupling', i.e. first identify the most useful couplings to create conceptual coupled models
- Ask the CSDMS community through surveys: what types of social issues are you interested in? How can we translate your ideas into something usable?

#### 2. Issues that emerge when trying to link social-earth systems dynamics models:

a. Temporal Scales (e.g., short term human land use decisions can have long term geological process impacts)

- Momentary: seconds/days
- Local decision time frame (1-5 yrs): length to get a typical short-term return
- Typical "planning" time frame (5-15 yrs): the length of most economic, etc., forecasts

- A governmental/planning "long term" time frame (25-50yrs): about a single generation, maximum length of a human memory
- Archaeological time scales (100's-1000's of yrs): length of a "civilization", length of written or social memory
- Geologic time scales (1000's 100,000's of yrs): length of human evolution

b. Spatial scales (e.g., focus on household, community decision-making processes and geological processes). The time and space dynamics studied depends on the questions being asked. It is not something the FRG should put constraints on. Identification of scales relevant to coupled Human Dimension + Earth System Models: (e.g. 'like can only be coupled with like')

- Watershed: Single medium-sized community or series of very small communities (e.g., farming hamlets); Single society/civilization; External social/economic influences possible/likely from larger scale social phenomena
- Flood plain: Large-small communities, single to medium-small network of communities; Typically single society/civilization, but possible for multiple (e.g., city-states); Can be connected to larger social phenomena, or self-contained (though typically connected externally in some ways); Regional system of watersheds, rivers, floodplains; Network of communities (various possible hierarchy/heterarchies possible); Typically single society/civilization, but possible for multiple (e.g., city-states); Likely "self"-contained, but certainly can be connected outwardly (esp. inter-regional trade)
- Continental: Multiple communities, various sizes; Multiple networks/societies/civilizations; More likely to be "Self" contained, again could be connected to global scale networks
- Global: Many networks/societies/civs of many sizes; Self-contained on spaceship earth.

## 3. Identification of interconnection of social and geodynamic models (not comprehensive)

- Changes to vegetation: Anthropogenic impacts of grazing, farming, woodcutting, burning, change in biodiversity/ecosystem services
- Direct Interaction with flow:\_Earthworks such as terraces, checkdams, bulwarks, levees, ditches, canals, etc.
- Manipulation of substrate: Change to soil organic matter affects infiltration, veg. growth, etc.

## 4. Goals of the coupled modeling system: academic vs. practical

Academic-geared models could be used as the base for applied models: user-directed, i.e. asking what a certain community needs, then build a model to address those needs—(bottom-up) OR I've got a cool model of marbles rotating in a drum; how can this be applied to improve conditions for some community (top-down)? If you come to stakeholders or policy makers with solutions derived purely from academic speculations, then your response may be suspect. Using a bottom-up approach engages the stakeholders and end-users of the model results. Bottom-up organization is important, but may not be an efficient approach for our present model developers, thus the need to ask CSDMS members to identify the potential human dimension of their models.

- Academic: Increase our understanding of the interaction and dynamics of coupled systems in general; Experimentation of coupling, model simplification, etc.; Study generalized processes could be in various places/times; Variety of time-scales and spatial scales; only need general methods/expertize; Validity/validation important, but mainly to justify the insights gained as "real"; Applications to case-studies mainly just as examples
- Practical/Applied: Help for a particular problem in a particular place; Specific spatial and temporal; Validity is very important (real decisions will be based on the model output); Require specific expertise and method; Focus on specific problems and processes

## 5. Agent-based Models

- ABMs are simple, can be used easily to show policy makers how agents may respond under certain conditions
- Need a set of generic rules so that ABMs can be linked to existing models. What components can be translated from code to a more 'generic' form for coupling?
- How to scale or connect time stepping of human/social processes to landscape evolution (LSE) timescales? Can use a bridging model to 'harmonize' between ABM models and land surface dynamics models

## 6. Other Questions/Observations:

- What is the social relevance of each of the models already in the CSDMS?
  - Need a system for identifying possible linkages and human components in existing models in the repository
  - Create a classification scheme for existing CSDMS models that may be combined with appropriately scaled social dynamics models (e.g. pollution in a stream system vs. collapse of societies).
- What models available through ComSES (open sourced ABM community: <u>http://www.openabm.org/comses</u>) can be componentized in a reusable way for coupling to land surface process models?
- How to handle uncertainty in these models? Hard to get at one solution is to create multiple working hypotheses, test using several models, then toss out those that appear to be wrong. Same Process of Elimination, can be used to help identify which models would be appropriate for coupling
- Is the modular approach most practical?
- How do you simplify the process? The models do not have to functioning at the same rate
- How do you test for validity? Can you compare social models? Presently, not a means of testing for validity. Could look at decision-making models, but each discipline (economics, psychology) has their own models. What is the decision making process for which model to choose? Which model matches the empirical data? Establish generic rules!
- Do not need to separate spatially-explicit models and numerical models, but be explicit about the inputs.
- Look at examples that have been successful in the past, e.g. Enkimdu Simulation Framework: (https://oi.uchicago.edu/OI/PROJ/MASS/papers/BrazilSFI2005\_Rev1\_SHORT.pdf)

## 6.11 Critical Zone Focus Research Group

**Overview:** The focus during the first year has been to think through a strategy and a way forward for advancing development, sharing and documenting of models that are used in Critical Zone research. Our CZFRG team has been carrying on informal discussions with CZ scientists and through formal participation in national and international workshops. Major workshops are listed below. The Critical Zone has become an encompassing theme for the Earth surface experimental research through the NSF Critical Zone Observatory program <a href="http://criticalzone.org/national">http://criticalzone.org/national</a>, the European CZ initiative <a href="http://www.soiltrec.eu/events/events.html">http://www.soiltrec.eu/events/events.html</a> and a new CZ research program in China (Geobiology, 2012). The CZFRG team has participated in a wide range of research efforts, workshops and national meetings to begin the process. One of our first efforts has been to try to capture the range of models that are used by CZ scientists. The "mindmap" below (Fig. 8) was developed by Duffy and Li to express the wide range of models that are currently being developed.



Figure 9 Mindmap of CSDMS-CZO related models

**Integrated Modeling:** The Critical Zone (CZ) incorporates all aspects of the earth's environment from the vegetation canopy to the bottom of groundwater. CZ researchers target processes that cross timescales from that of water fluxes (milliseconds to decades) to that of the evolution of landforms (thousands to tens of millions of years). Conceptual and numerical models are used to investigate the important fluxes: water, energy, solutes, carbon, nitrogen, and sediments. Depending upon the questions addressed, these models must calculate the distribution of landforms, regolith structure and chemistry, biota, and the chemistry of water, solutes, sediments, and soil atmospheres. No single model can accomplish all these objectives. A group of scientists at Penn State are designing and developing model capabilities to explore the CZ and testing them at the Susquehanna Shale Hills CZ Observatory. To examine processes over different timescales, we establish the core hydrologic fluxes using the Penn State Integrated Hydrologic Model (PIHM) – and then augment PIHM with simulation modules. For example, most land-atmosphere models currently do not incorporate an accurate representation of the geologic subsurface. We are exploring what aspects of subsurface structure must be accurately modeled to simulate water, carbon, energy, and sediment fluxes accurately. Only with a suite of modeling tools will we learn to forecast – earthcast -- the future CZ. Paper presented at: Geochemistry of the Earth's Surface meeting, GES-10, and published Duffy et al, (2014).

#### Social Computing

The NSF EarthCube GEOSOFT project was fully funded this year (2013-2016). Yolanda Gil (USC) is the PI and Scott Peckham (CSDMS), Chris Duffy (Penn State), and Chris Mattman (JPL) are co-PI's. Although scientists program a lot of code to analyze their data, this software is often not shared and rarely preserved. The GeoSoft project brings together computer scientists, geoscientists, and social scientists to develop computational tools for documenting and sharing code and explore better ways for scientists to receive credit for their model and data development. GeoSoft is a social collaboration site where scientists can discover alternative approaches to free software, use intelligent interfaces to explain how their software works, and form productive communities around software projects. This research has the potential to fundamentally

transform geosciences by making scientific software readily available to researchers and citizen scientists for efficient data analysis. (http://www.isi.edu/ikcap/geosoft/)

### Model-Integration and Collaboration across Earth Science Domains

In this recently funded NSF effort through the NSF INSPIRE program (Duffy, Gil and Hanson) we are attempting to use on-line technology as a means of sharing models, developing model-coupling strategies and for integrating models with experimental data. The concept uses MediaWiki and SemanticWiki as framework for sharing, setting up tasks, and in general creating a collaborative on-line framework for developing predicitive tools for that span Earth science research domains. (for details see: http://www.organicdatascience.org)

### Funded projects

1. NSF EarthCube Building Blocks: GeoSoft: Software Stewardship for the Geosciences. NSF ICER, *Integrative and Collaborative Education and Research*, (2013-2016), Yolanda Gil (PI), Christopher Duffy (Co-PI), Scott Peckham (Co-PI), Christ Mattmann (Co-PI), Erin Robinson (Co-PI), \$750,00.

2. NSF INSPIRE Track 1: The Age of Water and Carbon in Hydroecological Systems: A New Paradigm for Science Innovation and Collaboration through Organic Team Science, (2013-2016) Chris Duffy, Yolanda Gil USC, Paul Hanson UW, \$1,000,000.

## References

2nd International Geobiology Conference: critical zone observatories for sustainable soil development and beyond and SoilTrEC Stakeholder and Training Event, Wuhan, China, 4th to 8th September 2012.

C Duffy, Y Shi, K Davis, R Slingerland, L Li, PL Sullivan, Y Goddéris, SL Brantley, Designing a Suite of Models to Explore Critical Zone Function, Procedia, Earth and Planetary Sciences, in press.

## 7.0 CSDMS2.0 Year 2 Priorities and Management of Resources

The CSDMS budget resources are roughly divided into four components:

1) 25% supporting middleware development (e.g. WMT plug-and-play environment, BMI and CMI interface standards, semantics, support services),

2) 25% supporting community networking, capacity building and working group activities (e.g. developing the model repository, metadata),

3) 25% supporting CSDMS support services (e.g. HPCC operations, model simulations, data handling, and other modeling services), and

4) 25% supporting education and knowledge products (e.g. model algorithms, numerical techniques, clinics, and short courses).

This division of resources is considered optimal for the CSDMS mission.

CSDMS Integration Facility Staff continue to juggle the competing demands of an actively engaged and evergrowing CSDMS Community. CSDMS staff continues their community interactions at both national and international venues. Expenditures related to the Integration Facility staff, travel expenses related to CSDMS governance, operations and workshop participation costs are provided below in Section 8.0. Priorities for Year 8 will continue to be responsive to the active CSDMS communities. This includes focusing on developments in the social dynamics of operating a large community effort, getting more contributed models able to work within CMT, producing a well-vetted CSDMS state-of-the-art special issue of C&G, streamlining the component wrapping process for model developers, and further develop educational tools and products for advancing computational approaches to earth-surface dynamics.

## 7.1 CSDMS2.0 Year 3 Goals — CSDMS Portal

## a) CSDMS transfer of model repository

For over 6 years, CSDMS has been successfully archiving and hosting source code of numerical models through the software versioning and revision control system, Subversion; currently locally maintained on the CSDMS webserver. This centralized repository service is made available to all earth surface model developers. However, CSDMS would like to move to the hosting service GitHub. GitHub provides a Web-based graphical interface through which, for example, people could 'fork' a model repository (copy a repository from one user's account to another), make local changes and then share the changes with the original owner by a so-called "pull request". Through the web, with the click of a button the original owner can accept the suggested changes, and they become integrated into the main code. This way, modeling teams can work more efficiently, and managing the code is more transparent. Through GitHub, source code will get more exposure, so models might be used more. The advantage for CSDMS-IF is that the facility has to spend fewer resources in maintaining the local version control system. GitHub is free for open source software projects. The main efforts to transfer to GitHub are: 1) guaranty that model DOIs are pointing to the right version of source code and that those versions cannot be modified; 2) Integration with the CSDMS website and GitHub. CSDMS has set up its current version control system such that a model download request done through the CSDMS website directly accesses the model repository subversion to find all the source code files and place them on a ftp server, after which a link is provided in the webpage so the requester can download the code. Similar functionality will be built for GitHub as well. 3) Model download information.

## b) Fully integrate JSXGraph functionality

The CSDMS website has the functionality to plot functions, which makes it possible to provide comprehensive information on models and their simulations to help new users better understand key functions of models. We will integrate this functionality for most of the labs as well as for the help pages of the modules that are available in the WMT.

### c) Document model animations of key processes

For educational purposes, CSDMS would like to build a library of short individual model animations that highlight the different key processes of a model. This will make it easier to understand the importance of certain processes in a model and how they might influence simulation results. Several models will be selected and animations will be set up in close collaboration with the model developer. The animations can be part of the educational repository to use for courses.

**Milestones**: A) Transfer the model repository into GitHub. Integrate the GitHub repository in the CSDMS website so versions of source code can be viewed through the CSDMS website and all version of the source code can easy be downloaded through the CSDMS website. B) Integrate JSXGraph functionality into the lab and WMT model help pages. C) Develop an animation library of key model processes.

**Resources:** 0.5 FTE Web Specialist.

## 7.2 CSDMS 2.0 Year 3 Goals—Cyber Plans

In the coming year, the CSDMS IF software engineers will primarily focus on three tasks:

1. Create a model uncertainty service component for WMT using Sandia National Laboratories' DAKOTA software.

2. Create a WMT service component for standard names.

3. Continue to wrap models in the CSDMS repository with BMI and make them available in WMT.

**Model uncertainty service component**. The DAKOTA Project has developed an extensive set of opensource, component-based tools for analyzing model uncertainty in an HPC environment that are well-suited for the CSDMS modeling framework. DAKOTA is designed to address the issues of uncertainty quantification, sensitivity analysis, optimization, and calibration (parameter estimation). DAKOTA operates by assuming full, low-level control of a model by connecting through an interface similar to the CSDMS BMI. Once connected, DAKOTA runs a model numerous—possibly thousands of—times with different settings in order to converge on a solution for a requested analysis. The CSDMS staff will create a service component for DAKOTA and incorporate it into WMT. Because of the possibility of prohibitively long run times with DAKOTA, we will focus, at this point, on ensuring the service component works for models that produce 0D (point or time series) output. We will also explore other strategies for quantifying model uncertainty, including adding the USGS UCODE package, as well as other benchmark or unit tests that can be made available through WMT.

### Milestones:

- 1. Install DAKOTA on the CSDMS HPCC, beach.colorado.edu, and use its command line interface to perform an analysis on a single model in the CSDMS repository, such as HydroTrend.
- 2. Write a service component to incorporate the DAKOTA tools.
- 3. Devise a GUI for generically representing the inputs to the DAKOTA tools; implement the GUI, and the service component above, in WMT.
- 4. Test, and iteratively refine, the DAKOTA service component on all component models that produce 0D output that are currently available in WMT.

**Resources:** 1.25 FTE software engineer.

Standard names service component. Across the earth sciences (e.g., the NSF EarthCube initiative), one of the biggest challenges in developing "seamless" data and modeling systems is *semantic mediation*. Each scientific discipline has a large amount of specialized, non-standardized, terminology (e.g., names for physical quantities, species). When automated systems share data, it is essential to have a robust method for defining standardized terminology to be used throughout the system. CSDMS has started to use standards from the

CF conventions to provide well-defined standard names for different physical quantities and for inclusion as metadata within NetCDF files to facilitate sharing of data. CSDMS is also working with the controlled vocabulary for hydrologic models developed by the CUAHSI-HIS project, and has adopted Unidata's UDUNITS standard for measurement units. In the coming year, the CSDMS staff will work, with assistance from its domain-specific working groups, to integrate semantic mediation databases into the CSDMS modeling framework as a service component that can be used in WMT.

### Milestones:

- 1. Incorporate the CSDMS standard names Python package into the coupling framework.
- 2. Develop web services for the standard names.
- 3. Expose component standard names through WMT uses/provides ports.

### **Resources:** 0.25 FTE software engineer.

**Wrap models with BMI**. The CSDMS IF software engineers will continue the ongoing effort of wrapping models in the CSDMS repository with a BMI. We will focus on models that were available in CMT, but aren't currently available in WMT, such as Erode, as well as models that have standardized outputs, such as MODFLOW, which will be helpful for implementing and testing the DAKOTA service component. Other candidates include: the collection of BoemSlip models (HurriSlip, SuspendiSlip, and TurbiSlip), Flexure, ROMS-lite, and selected Landlab components.

### Milestones:

- 1. Identify a set of candidate models and write BMI wrappers for them.
- 2. Ensure the new components work in WMT.

Resources: 0.25 FTE software engineer.

## 7.2.1 Supplemental work plan—BMI Builder

Because of the necessity for BMI in model coupling, we will develop tools to make it easier for model developers to *implement* and *test* a full BMI in their code. We will develop a "BMI Builder" that facilitates the process of implementing a BMI for an existing model, thus making it a couplable component in the CSDMS modeling framework. The BMI Builder will consist of a command-line tool for collecting information about a model and a code generator that takes this information and creates a series of template files that containing BMI definitions for the model. The model developer will then edit the template files to add model-specific code. The BMI builder will be designed with product user feedback, and documented through the CSDMS wiki. We plan on teaching a clinic on the BMI builder at the CSDMS annual meeting 2015. We will also develop a user-friendly version of the command-line tool as a Web application. Part of the developing process will be reserved for thoroughly testing the BMI Builder to identify and resolve potential bugs and enlarge users' convenience.

Milestones:

- 1. Build a command-line tool for collecting model information.
- 2. Write a code generator for creating BMI definitions.
- 3. Develop a web-based interface to collect model information and deliver resulting template files.

Resources: 0.25 FTE software engineer; 0.08 FTE web specialist, EKT specialist 0.08 FTE (1 month)

# 7.3 CSDMS2.0 Year 3 — EKT Goals

- Document newly componentized models and maintain tight integration between WMT and Help system.
- Design and develop simple modeling labs with existing components
- Work with EKT WG members to merge existing stand-alone labs into the EKT repository.
- Facilitate Science-on-a-Sphere contributions from community members.
- Develop advanced modeling labs with new components coming online Expand animations repository (e.g. vegetation and sediment processes).
- A focused EKT case study will be employed with the new ROMS-LITE component. This includes development of several student labs focused on nearshore processes and marine sediment transport dynamics (in collaboration with Courtney Harris, VIMS). We plan to beta-test the package in another classroom in collaboration with Sam Bentley, LSU.
- Teach clinics on earth surface process modeling and teaching (at CSDMS annual meeting, NCED summer institute).
- Maintain existing knowledge transfer efforts for the CSDMS community (i.e. presentations for industry representatives and policy-makers).

## Milestones:

- 1. Increase the use of WMT
- 2. Complete documentation and associated modeling lab for each new WMT component
- 3. Develop new ROMS-Lite educational module, test and evaluate this modules with students in independent classroom.

Resources: EKT specialist 0.5 FTE, SE 0.08 FTE

## 8.0 NSF Revenue & Expenditure (\$K with rounding errors)

	Est. <b>\$</b> K	Est. <b>\$</b> K
	Year 6	Year 7
A. Salaries & Wages		
Executive Director:	\$57	\$56
Software Engineers:	\$144	\$164
Communication Staff*	\$100	\$100
Admin Staff**	\$72	<u>\$52</u>
Total Salaries	\$373	\$372
B. Fringe	\$113	\$111
D. Travel		
Center Staff:	\$10	\$15
Steering Committee	\$6	\$10
Executive Com.	<u>\$10</u>	<u>\$15</u>
Total Travel	\$26	\$40
E. Annual Meeting	\$70	\$72
F. Other Direct Costs		
Materials & Suppl	\$1	\$1
Publication Costs	\$2	\$1
Computer Services:	\$25	\$24
Non Capital Equipment	\$2	\$2
Communications	<u>\$3</u>	<u>\$3</u>
Total Other Costs	\$33	\$31
G. Total Direct Costs	\$615	\$626
H. Indirect Cost	\$286	\$291
I. Total Costs	\$900	\$917

#### Notes:

1) Estimates include salaries projected 3 months to the end of the CSDMS fiscal year.

2) \* Communication Staff includes Cyber + EKT Scientists

3) \*\* Admin Staff includes Executive Assistant + System Administrator + Accounting Technician.

4) CU completes a preliminary estimate of expenditures after 60 days of a time marker. CU provides a finalization typically within 90 days of a fiscal year.

#### Additional Funds Received by CSDMS IF Staff and Associates (see Section 2.4) Year 6:

NASA: Threatened River Delta Systems: \$143K, Accelerating Changes in Arctic River Discharge \$75K BOEM: Shelf-Slope Sediment Exchange, N Gulf of Mexico: Numerical Models for Extreme Events \$75K NSF: 1) Governance in Community Earth Science \$85K; 2) A Delta Dynamics Collaboratory \$126K, 3) River plumes as indicators of Greenland Ice Sheet Melt \$90K

U. Colorado: Salary support for the CSDMS Integration Facility: \$73K

## Year 7:

NASA: Threatened River Delta Systems: \$143K, Accelerating Changes in Arctic River Discharge \$75K BOEM: Shelf-Slope Sediment Exchange, N Gulf of Mexico: Numerical Models for Extreme Events \$75K NSF: 1) A Delta Dynamics Collaboratory \$126K, 2) River plumes as indicators of Greenland Ice Sheet Melt \$90K

U. Colorado: Salary support for the CSDMS Integration Facility: \$73K

## Appendix 1: Institutional Membership & Member Location Maps

U.S. Academic Institutions: 126 with 3 new members from July 2013 - July 2014

- 1. Arizona State University
- 2. Auburn University, Alabama
- 3. Binghamton University, New York
- 4. Boston College
- 5. Boston University
- 6. Brigham Young University, Utah
- California Institute of Technology, Pasadena
- 8. California State University Fresno
- 9. California State University Long Beach
- 10. California State University Los Angeles
- 11. Carleton College, Minneapolis
- 12. Center for Applied Coastal Research, Delaware
- 13. Chapman University, California
- 14. City College of New York, City University of New York
- 15. Coastal Carolina University, South Carolina
- 16. Colorado School of Mines, Colorado
- 17. Colorado State University
- 18. Columbia/LDEO, New York
- 19. Conservation Biology Institute, Oregon
- 20. CUAHSI, District of Columbia
- 21. Desert Research Institute, Nevada
- 22. Duke University, North Carolina
- 23. Florida Gulf Coast University
- 24. Florida International University
- 25. Franklin & Marshall College, Pennsylvania
- 26. George Mason University, VA
- 27. Georgia Institute of Technology, Atlanta
- 28. Harvard University
- 29. Idaho State University
- 30. Indiana State University
- 31. Iowa State University
- 32. Jackson State University, Mississippi
- 33. John Hopkins University, Maryland
- 34. Louisiana State University
- 35. Massachusetts Institute of Technology
- 36. Michigan Technological University
- 37. Monterey Bay Aquarium Research Inst.
- 38. Murray State University
- 39. North Carolina State University
- 40. Northern Arizona University
- 41. Northern Illinois University
- 42. Northwestern University
- 43. Nova Southeastern University, Florida
- 44. Oberlin College
- 45. Ohio State University
- 46. Oklahoma State University
- 47. Old Dominion University, Virginia
- 48. Oregon State University
- 49. Penn State University
- 50. Portland State University

- 51. Purdue University, Indiana
- 52. Rutgers University, New Jersey
- 53. San Jose State University
- 54. Scripps Institution of Oceanography, CA
- 55. South Dakota School of Mines, South Dakota
- 56. Stanford, CA
- 57. State University (Virginia Tech), VA
- 58. Syracuse University, New York
- 59. Texas A&M, College Station, TX
- 60. Texas Christian University
- 61. Tulane University, New Orleans
- 62. United States Naval Academy, Annapolis
- 63. University of Alabama Huntsville
- 64. University of Alaska Fairbanks
- 65. University of Arkansas
- 66. University of Arizona
- 67. University of California Berkeley
- 68. University of California Davis
- 69. University of California Irvine
- 70. University of California Los Angeles
- 71. University of California San Diego
- 72. University of California -Santa Barbara
- 73. University of California Santa Cruz
- 74. University of Colorado Boulder
- 75. University of Connecticut
- 76. University of Delaware
- 77. University of Florida
- 78. University of Houston
- 79. University of Idaho
- 80. University of Illinois-Urbana Champaign
- 81. University of Iowa
- 82. University of Kansas
- 83. University of Louisiana Lafayette
- 84. University of Maine
- 85. University of Maryland, Baltimore County
- 86. University of Memphis
- 87. University of Miami
- 88. University of Michigan
- 89. University of Minnesota Minneapolis
- 90. University of Minnesota Duluth
- 91. University of Nebraska Lincoln
- 92. University of Nevada Reno
- 93. University of New Hampshire
- 94. University of New Mexico
- 95. University of New Orleans

98.

99.

100.

101.

102.

- 96. University of North Carolina Chapel Hill
- 97. University of North Carolina Wilmington

University of Pennsylvania - Pittsburgh

48

University of North Dakota

University of Oklahoma

University of Pittsburgh

University of Oregon

- 103. University of Rhode Island
- 104. University of South Carolina
- 105. University of South Florida
- 106. University of Southern California
- 107. University of Tennessee Knoxville
- 108. University of Texas Arlington
- 109. University of Texas Austin
- 110. University of Texas El Paso
- 111. University of Texas San Antonio
- 112. University of Utah
- 113. University of Virginia
- 114. University of Washington

#### U.S. Federal Labs and Agencies: 21 as of July 2014

- 1. Argonne National Laboratory (ANL)
- 2. Idaho National Laboratory (IDL)
- 3. National Aeronautics & Space Administration (NASA)
- 4. National Center for Atmospheric Research (NCAR)
- 5. National Oceanographic Partnership Program (NOPP)
- 6. National Science Foundation (NSF)
- 7. Oak Ridge National Laboratory (ORNL)
- 8. Sandia National Laboratories (SNL)
- 9. U.S. Dept. of Agriculture (USDA)
- 10. U.S. DoC National Oceanic & Atmospheric Administration (NOAA)

- 115. University of Wyoming
- 116. Utah State University
- 117. Vanderbilt University
- 118. Villanova University, Pennsylvania
- 119. Virginia Institute of Marine Science (VIMS)
- 120. Virginia Polytechnic Institute, VA
- 121. Washington State University
- 122. West Virginia University
- 123. Western Carolina University
- 124. Wichita State University
- 125. William & Mary College, VA
- 126. Woods Hole Oceanographic Inst.
- 11. U.S. DoC National Weather Service (NWS)
- 12. U.S. DoD Naval Research Laboratory (NRL)
- 13. U.S. DoD Office of Naval Research (ONR)
- 14. U.S. DoD Army Corps of Engineers (ACE)
- 15. U.S. DoD Army Research Office (ARO)
- 16. U.S. DoI Bureau of Ocean Energy Management (BOEM)
- 17. U.S. DoI Bureau of Reclamation
- 18. U.S. DoI Geological Survey (USGS)
- 19. U.S. DoI National Forest Service (NFS)
- 20. U.S. DoI National Park Service (NPS)
- 21. U.S. Nuclear Regulatory Commission (NRC)

#### U.S. Private Companies: 25 with 3 new members from July 2013-July 2014

- 1. Airlink Communications, Hayward CA
- 2. Aquaveo LLC, Provo, Utah
- 3. ARCADIS-US, Boulder, Colorado
- 4. Chevron Energy Technology, Houston, TX
- 5. ConocoPhillips, Houston, TX
- 6. Deltares, USA
- 7. Dewberry, Virginia
- 8. DHI, Solana Beach, CA
- 9. Everglades Partners Joint Venture (EPJV), Florida
- 10. ExxonMobil Research & Engineering, Houston TX
- 11. Geological Society of America Geocorps
- 12. Idaho Power, Boise
- 13. PdM Calibrations, LLC, Florida
- 14. Philip Williams and Associates, Ltd., California

- 15. Schlumberger Information Solutions, Houston, TX
- 16. Science Museum of Minnesota, St. Paul, MN
- 17. Shell USA, Houston, TX
- 18. Stratus Consulting, Boulder, CO
- 19. Stroud Water Research Center, Avondale, PA
- 20. Subsurface Insights, Hanover, NH
- 21. URS-Grenier Corporation, Colorado
- 22. Warren Pinnacle Consulting, Inc., Warren, VT
- 23. The Von Braun Center for Science & Innovation Inc
- 24. The Water Institute of the Gulf, Louisiana
- 25. UAN Company

Foreign Membership: Current total of 292 with 17 of them being new members from May 2013-present. (66 countries outside of the U.S.A.: Algeria, Argentina, Armenia, Australia, Australia, Bangladesh, Belgium, Bolivia, Brazil, Bulgaria, Cambodia, Canada, Chile, China, Colombia, Cuba, Denmark, Egypt, El Salvador, France, Germany, Ghana, Greece, Hong Kong, Hungary, India, Indonesia, Iran, Iraq, Ireland, Israel, Italy, Japan, Jordan, Kenya, Malaysia, Mexico, Morocco, Myanmar, Nepal, Netherlands, New Zealand, Nigeria, Norway, Pakistan, Peru, Philippines, Poland, Portugal, Qatar, Romania, Russia, Saudi Arabia, Scotland, Singapore, South Africa, South Korea, Spain, Sweden, Switzerland, Taiwan, Thailand, Netherlands, Turkey, UK, United Arab Emirates, Uruguay, Venezuela, Việt Nam).

Foreign Academic Institutes: 190 with 14 new members as of July 2014

- 1. Aberystwyth University, Wales, UK
- 2. Adam Mickiewicz University (AMU) Poznan, Poland
- 3. AGH University of Science and Technology, Krakow, Poland
- 4. AgroCampus Ouest, France
- 5. Aix-Marseille University, France
- 6. Anna University, India
- 7. ANU College, Argentina
- 8. Architectural Association School of Architecture, UK
- 9. Aristotle University of Thessaloniki, Greece
- 10. Bahria University, Islamabad, Pakistan
- 11. Bangladesh University of Engineering and Technology, Dhaka, Bangladesh
- 12. Birbal Sahni Institute of Palaeobotany, India
- 13. Bonn University, Germany
- 14. Blaise Pascal University, Clermont, France
- 15. Brandenburg University of Technology (BTU), Cottbus, Germany
- 16. British Columbia Institute of Technology (BCIT), Canada
- 17. Cardiff University, UK
- 18. Carleton University, Canada
- 19. Chengdu University of Technology, China
- 20. China University of Geosciences- Beijing, China
- 21. China University of Petroleum, Beijing, China
- 22. Christian-Albrechts-Universitat (CAU) zu Kie, Germany
- 23. CNRS / University of Rennes I, France
- 24. Cracow University of Technology, Poland
- 25. Dalian University of Technology, Liaoning, China
- 26. Darmstadt University of Technology, Germany
- 27. Delft University of Technology, Netherlands
- 28. Democritus University of Thrace, Greece
- 29. Diponegoro University, Semarang, Indonesia
- 30. Dongguk University, South Korea
- 31. Durham University, UK
- 32. Ecole Nationale Superieure des Mines de Paris, France
- 33. Ecole Polytechnique, France
- Eidgenossische Technische Hochschule (ETH) Zurich, Switzerland

- 35. FCEFN-UNSJ-Catedra Geologia Aplicada II, Argentina
- 36. Federal Ministry of Environment, Nigeria
- 37. Federal University of Itajuba, Brazil
- 38. Federal University of Petroleum Resources, Nigeria
- 39. Federal University Oye-Ekiti, Nigeria
- 40. First Institute of Oceanography, SOA, China
- 41. Free University of Brussels, Belgium
- 42. Guanzhou University, Guanzhou, China
- 43. Heriot-Watt University, Edinburgh, UK
- 44. Hohai University, Nanjing, China
- 45. Hong Kong University, Hong Kong
- 46. IANIGLA, Unidad de Geocriologia, Argentina
- 47. Imperial College of London, UK
- 48. India Institute of Technology Bhubaneswar, India
- 49. India Institute of Technology Delhi
- 50. India Institute of Technology Kanpur
- 51. India Institute of Technology Madras
- 52. India Institute of Technology Mumbai
- 53. Indian Institute of Science Bangalore
- 54. Indian Institute of Technology- Bombay
- 55. Institut Univ. Europeen de la Mer (IUEM), France
- 56. Institute of Engineering (IOE), Nepal
- 57. Institute of Geology, China Earthquake Administration
- 58. Instituto de Geociencias da Universidade Sao Paulo (IGC USP), Brasil
- 59. Kafrelsheikh University, Kafrelsheikh, Egypt
- 60. Karlsruhe Institute of Technology (KIT), Germany
- 61. Katholieke Universiteit Leuven, KUT, Belgium
- 62. King's College London, UK
- 63. King Fahd University of Petroleum and Mineral, Saudi Arabia
- 64. Kocaeli University, Izmit, Turkey
- 65. Lanzhou University, China
- 66. Leibniz-Institute fur Ostseeforschung Warnemunde (IOW)/Baltic Sea Research, Germany
- 67. Leibniz Universitat Hannover, Germany
- 68. Loughborough University, UK
- 69. Lund University, Sweden
- 70. McGill University, Canada
- 71. Mohammed V University-Agdal, Rabat, Morocco
- 72. Mulawarman University, Indonesia
- 73. Nanjing University of Information Science & Technology (NUIST), China

- 74. Nanjing University, China
- 75. National Cheng Kong University
- 76. National Taiwan University, Taipei, Taiwan
- 77. National University (NUI) of Maynooth, Kildare, Ireland
- 78. National University of Sciences & Technology, Pakistan
- 79. National University of Sciences & Technology, (NUST), Pakistan
- 80. Natural Resources, Canada
- 81. Northwest University of China, China
- 82. Norwegian University of Life Sciences, Norway
- 83. Ocean University of China, China
- 84. Padua University, Italy
- 85. Peking University, China
- 86. Pondicherry University, India
- 87. Pukyong National University, Busan, South Korea
- Royal Holloway University of London, UK
- 89. Sejong University, South Korea
- 90. Seoul National University, South Korea
- 91. Shihezi University, China
- 92. Singapore-MIT Alliance for Research and Technology (SMART), Singapore
- 93. Southern Cross University, United Arab Emirates (UAE)
- 94. Sriwijaya University, Indonesia
- 95. SRM University, India
- 96. Stockholm University, Sweden
- 97. Tarbiat Modares University, Iran
- 98. The Maharaja Sayajirao University of Baroda, India
- 99. Tianjin University, China
- 100. Tsinghua University, China
- 101. Universidad Agraria la Molina, Peru
- 102. Universidad Complutense de Madrid, Spain
- 103. Universidad de Granada, Spain
- 104. Universidad de Guadalajara, Mexico
- 105. Universidad de la Republica, Uruguay
- 106. Universidad de Oriente, Cuba
- 107. Universidad de Zaragoza, Spain
- 108. Universidad Nacional de Catamarca, Argentina
- 109. Universidad Nacional de Rio Negro, Argentina
- 110. Universidad Nacional de San Juan, Argentina
- 111. Universidad Politecnica de Catalunya, Spain
- 112. Universidade de Lisboa, Lisbon, Portugal
- 113. Universidade de Madeira, Portugal
- 114. Universidade do Minho, Braga, Portugal

- 115. Universidade Federal do Rio Grande do Sul (FRGS), Brazil
- 116. Universit of Bulgaria (VUZF), Bulgaria
- 117. Universita "G. d'Annunzio" di Chieti-Pescara, Italy
- 118. Universitat Potsdam, Germany
- 119. Universitat Politecnica de Catalunya, Spain
- 120. Universitas Indonesia, Indonesia
- 121. Universite Bordeaux 1, France
- 122. Universite de Rennes (CNRS), France
- 123. Universite du Quebec a Chicoutimi (UQAC), Canada
- 124. Universite Joseph Fourier, Grenoble, France
- 125. Universite Montpellier 2, France
- 126. Universiteit Gent, Ghent, Belgium
- 127. Universiteit Stellenosch University, South Africa
- 128. Universiteit Utrecht, Netherlands
- 129. Universiteit Vrije (VU), Amsterdam, Netherlands
- 130. Universiti Teknologi Mara (UiTM), Mayalsia
- 131. Universiti Malaysia Pahang, Malaysia
- 132. University College Dublin, Ireland
- 133. University of Bari, Italy
- 134. University of Basel, Switzerland
- 135. University of Bergen, Norway
- 136. University of Bremen, Germany
- 137. University of Brest, France
- 138. University of Bristol, UK
- 139. University of British Columbia, Canada
- 140. University of Calgary, Canada
- 141. University of Cambridge, UK
- 142. University of Cantabria, Spain
- 143. University of Copenhagen, Denmark
- 144. University of Dhaka, Bangladesh
- 145. University of Dundee, UK
- 146. University of Edinburgh, Scotland
- 147. University of Edinburgh, UK
- 148. University of Exeter, UK
- 149. University of Ghana, Ghana
- 150. University of Guelph, Canada
- 151. University of Haifa, Israel
- 152. University of Ho Chi Minh City
- 153. University of Kashmir, India
- 154. University of Lethbridge, Canada
- 155. University of Manchester, UK
- 156. University of Malaya, Kuala Lumpur, Malaysia
- 157. University of Milano-Bicocca, Italy
- 158. University of Natural Resources & Life Sciences, Vienna, Austria
- 159. University of New South Wales, Australia
- 160. University of Newcastle upon Tyne, UK
- 161. University of Newcastle, Australia

- 162. University of Nigeria, Nsukka, Nigeria
- 163. University of Palermo, Italy
- 164. University of Padova, Italy
- 165. University of Pavia, Italy
- 166. University of Postdam, Germany
- 167. University of Queensland (UQ), Australia
- 168. University of Reading, Berkshire, UK169. University of Rome (INFN)"LaSapienza", Italy
- 170. University of Science Ho Chi Minh City, Viet Nam
- 171. University of Southampton, UK
- 172. University of St. Andrews, UK
- 173. University of Sydney, Australia
- 174. University of Tabriz, Iran
- 175. University of Tehran, Iran
- 176. University of the Philippines, Manila, Philippines
- 177. University of the Punjab, Lahore, Pakistan

#### **Foreign Private Companies:**

- 1. Aerospace Company, Taiwan
- 2. ASR Ltd., New Zealand
- 3. Bakosurtanal, Indonesia
- 4. BG Energy Holdings Ltd., UK
- 5. Cambridge Carbonates, Ltd., France
- 6. Deltares, Netherlands
- 7. Digital Mapping Company, Bangladesh
- 8. Energy & Environment Modeling, ENEA/UTMEA, Italy
- 9. Environnement Illimite, Inc., Canada
- 10. Excurra & Schmidt: Ocean, Hydraulic, Coastal and Environmental Engineering Firm, Argentina
- 11. Fugro-GEOS, UK
- 12. Geo Consulting, Inc., Italy
- 13. Grupo DIAO, C.A., Venezuela
- 14. Haycock Associates, UK
- 15. H.R. Wallingford, UK
- 16. IH Cantabria, Cantabria, Spain
- 17. InnovationONE, Nigeria
- 18. Institut de Physique de Globe de Paris, France
- 19. Institut Francais du Petrole (IFP), France
- 20. Jaime Illanes y Asociados Consultores S.A., Santiago, Chile
- 21. METEOSIM, Spain
- 22. MUC Engineering, United Arab Emirates (UAE)
- 23. Petrobras, Brazil
- 24. Riggs Engineering, Ltd., Canada
- 25. Saipem (oil and gas industry contractor), Milano, Italy
- 26. Shell, Netherlands
- 27. SEO Company, Indonesia
- 28. Statoil, Norway
- 29. Tullow Oil, Ireland
- 30. Vision on Technology (VITO), Belgium

#### Foreign Government Agencies: 72 as of July 1014

- 1. Agency for Assessment and Application of Technology, Indonesia
- 2. Bedford Institute of Oceanography, Canada

- 178. University of Waikato, Hamilton, New Zealand
- 179. University of Warsaw, Poland
- 180. University of West Hungary Savaria Campus, Hungary
- 181. University of Western Australia, Australia
- 182. Victoria University of Wellington, New Zealand
- 183. VIT (Vellore Institute of Technology) University, Tamil Nadu, India
- 184. VUZF University, Bulgaria
- 185. Wageningen University, Netherlands
- 186. Water Resources University, Hanoi, Viet Nam
- 187. Wuhan University, Wuhan, China
- 188. Xi-an University of Architecture & Technology, China
- 189. York University, Canada
- 190. Zhejiang University, China

- 3. Bhakra Beas Management Board (BBMB), Chandigarh, India
- 4. British Geological Survey, UK
- 5. Bundesanstalt fur Gewasserkunde, Germany
- 6. Bureau de Recherches Géologiques et Minières (BRGM), Orleans, France
- 7. Cambodia National Mekong Committee (CNMC), Cambodia
- 8. Center for Petrographic and Geochemical Research (CRPG-CNRS), Nancy, France
- 9. CETMEF/LGCE, France
- 10. Channel Maintenance Research Institute (CMRI), ISESCO, Kalioubia, Egypt
- 11. Chinese Academy of Sciences Cold and Arid Regions Environmental and Engineering Research Institute
- 12. Chinese Academy of Sciences Institute of Mountain Hazards and Environment, China
- 13. Chinese Academy of Sciences Institute of Tibetan Plateau Research (ITPCAS), China
- 14. Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia
- 15. Consiglio Nazionale delle Ricerche (CNR), Italy
- 16. French Agricultural and Environmental Research Institute (CEMAGREF)
- 17. French Research Institute for Exploration of the Sea (IFREMER), France
- 18. Geological Survey of Canada, Atlantic
- 19. Geological Survey of Canada, Pacific
- 20. Geological Survey of Israel, Jerusalem, Israel
- 21. Geological Survey of Japan (AIST), Japan
- 22. Geosciences, Rennes France
- 23. GFZ, German Research Centre for Geosciences, Potsdam, Germany
- 24. GNS Science, New Zealand
- 25. GNU VNIIGiM, Moscow, Russia
- 26. Group-T, Myanmar
- 27. Helmholtz Centre for Environmental Research (UFZ), Germany
- 28. Indian National Centre for Ocean Information Services (INCOIS), India
- 29. Indian Space Research Organization
- 30. Institut des Sciences de la Terre, France
- 31. Institut National Agronomique (INAS), Algeria
- 32. Institut Teknologi Bandung (ITB), Indonesia
- 33. Institute of Atmospheric Sciences and Climate (ISAC) of Italian National Research Council (CNR), Italy
- 34. Institute for Computational Science and Technology (ICST), Viet Nam
- 35. Institute for the Conservation of Lake Maracaibo (ICLAM), Venezuela
- 36. Institute of Earth Sciences (ICTJA-CSIC), Spain
- 37. Instituto Hidrografico, Lisboa, Lisbon, Portugal
- 38. Instituto Nacional de Hidraulica (INH), Chile
- 39. Instituto Nazionale di Astrofisica, Italy
- 40. International Geosphere Biosphere Programme (IGBP), Sweden
- 41. Iranian National Institute for Oceanography (INIO), Tehran, Iran
- 42. Italy National Research Council (CNR), Italy
- 43. Japan Agency for Marine-Earth Science Technology (JAMSTEC), Japan
- 44. Kenya Meteorological Services, Kenya
- 45. Korea Ocean Research and Development Institute (KORDI), South Korea
- 46. Korea Water Resources Corporation, South Korea
- 47. Lab Domaines Oceanique IUEM/UBO France
- 48. Laboratoire de Sciences de la Terre, France
- 49. Marine Sciences For Society, France
- 50. Ministry of Earth Sciences, India
- 51. Nanjing Hydraulics Research Institute, China
- 52. National Institute of Water and Atmospheric Research (NIWA), Auckland, New Zealand
- 53. National Research Institute of Science and Technology for Environment and Agriculture (CEMAGREF became IRSTEA), France
- 54. National Institute for Space Research (INPE), Brazil
- 55. National Institute of Oceanography (NIO), India
- 56. National Institute of Technology Rourkela, Orissa, India
- 57. National Institute of Technology Karnataka Surathkal, Mangalore, India
- 58. National Institute of Water and Atmosphere (NIWA), New Zealand

- 59. National Marine Environmental Forecasting Center (NMEFC), China
- 60. National Research Centre for Sorghum (NRCS), India
- 61. National Research Council (NRC), Italy
- 62. National Space Research & Development Agency, Nigeria
- 63. Qatar National Historic Environment Project
- 64. Scientific-Applied Centre on hydrometeorology & ecology, Armstatehydromet, Armenia
- 65. Senckenberg Institute, Germany
- 66. Shenzhen Inst. of Advanced Technology, China
- 67. South China Sea Institute of Technology (SCSIO), Guanzhou, China
- 68. The European Institute for Marine Studies (IUEM), France
- 69. The Leibniz Institute for Baltic Sea Research, Germany
- 70. UNESCO-IHE, Netherlands
- 71. Water Resources Division, Dept. of Indian Affairs and Northern Development, Canada
- 72. World Weather Information Service (WMO), Cuba

Independent Researchers (both U.S. and Foreign): 31 members self-identify either as independent researchers or left their affiliation unknown.

#### Membership Map



## Appendix 2: 2014 CSDMS Annual Meeting Abstracts (Keynotes and Posters)

Modeling hydrologic and erosional responses of landscapes to fire using the Landlab modeling environment

Jordan Adams, Tulane University New Orleans Louisiana, United States. jadams15@tulane.edu Nicole Gasparini, Tulane University New Orleans Louisiana, United States. Gregory Tucker, University of Colorado Boulder Colorado, United States. Erkan Istanbulluoglu, University of Washington Seattle Washington, United States. Eric Hutton, CSDMS Boulder Colorado, United States. Daniel Hobley, University of Colorado Boulder Colorado, United States. Sai Siddhartha Nudurupati, University of Washington Seattle Washington, United States.

Landscape response to fire has been well documented in field observations, but the effects beyond a single fire are not well understood. Utilizing models to understand this response through time is critical, as significant erosion events postfire could potentially disrupt steady- state landscapes and affect both short and long-term landscape evolution. Additionally, problems arise when climate change is also considered, as anthropogenic influences such as land use change or fire cessation programs have actually exacerbated fire recurrence. To understand and quantify landscape response to fire across multiple time scales, the Landlab modeling environment is used to explore the morphological impacts of erosion events post-fire. Landlab, a highly flexible plug-and-play modeling framework, can link together digital elevation model (DEM)-based grids, stochastic storm and fire generators, as well as overland flow and sediment transport modules to simulate scenarios that may cause large flow or erosion events in the first post-fire year. The parameters in these components are drawn from the existing post-fire literature and are applied across two grids of varying resolution. The coarser, 1-m DEM is from the Spring Creek watershed in Colorado, which burned in the 1996 Buffalo Creek fire and experienced significant erosion in the aftermath. The high-resolution 5-cm DEM from the Chiricahua Mountains in southeastern Arizona represents a small watershed that burned in the 2011 Horseshoe 2 fire, after which nearby sites experienced massive debris flows following a significant 5-year precipitation event. Both sites experienced the same intensity (I30 = 72 mm/hr) storm post-fire, but had significantly different erosional and hydrologic responses. The model will be validated using field data from the Spring Creek site, collected by the USGS several years post-fire, and then applied to the Chiricahua site. In addition to validating Landlab's suitability for post-fire modeling, the results can also shed light on what processes drive post-fire erosional responses across the different climate regimes of Colorado and Arizona, and how those responses may affect the morphology of these sites over much longer time scales.

#### A numerical modeling study of the effects of sediment properties on deltaic processes and morphology Rebecca Caldwell, *Indiana University*

We use numerical modeling to explain how deltaic processes and morphology are controlled by properties of the sediment input to the delta apex. We conducted 36 numerical experiments of delta formation varying the following sediment properties: median grain size, grain-size distribution shape, and percent cohesive sediment. As the dominant grain size increases deltas undergo a morphological transition from elongate with few channels to semi-circular with many channels. This transition occurs because the critical shear stress for erosion and the settling velocity of grains in transport set both the number of channel mouths on the delta and the dominant delta-building process. Together, the number of channel mouths and dominant process – channel avulsion, mouth bar growth, or levee growth – set the delta morphology. Coarse-grained, non-cohesive deltas have many channels that are dominated by avulsion, creating semi-circular planforms with relatively smooth delta fronts. Intermediate-grained deltas have many channels that are dominated by mouth bar growth, creating semi-circular planforms with smooth delta fronts. The process-based model presented here provides a previously lacking mechanistic understanding of the effects of sediment properties on delta channel network and planform morphology.

#### An immersed boundary method in Delft3D

Alberto Canestrelli, Penn State University University Park Pennsylvania, United States. <u>auc26@psu.edu</u> Rudy Slingerland, Penn State University University Park Pennsylvania, United States. <u>rxs15@psu.edu</u>

In this work an approach is proposed for solving the three dimensional shallow water equations with embedded boundaries that are not aligned with the underlying Cartesian grid. A hybrid cut-cell/ghost-cell method is proposed: ghost cells are used for the momentum equations in order to prescribe the correct boundary condition at the immersed boundary, while cut-cells are used in the continuity equation in order to conserve mass. The resulting scheme is robust and does not suffer any time step limitation for small cut cells. Comparisons toward analytical solutions and reference numerical solutions on curvilinear grids confirm the quality of the method.

#### A Simple Rule-Based Model for Distributary Networks

Dan Cazanacli, University of Minnesota Minneapolis Minnesota, United States. <u>cazanacli@yahoo.com</u> Matthew Wolinsky, Shell Technology Center Houston Texas, United States. Zoltan Sylvester, Shell Technology Center Houston Texas, United States. Alessandro Cantelli, Shell Technology Center, United States. Chris Paola, University of Minnesota Minneapolis Minnesota, United States.

Deltaic networks present a wide variation in almost any geomorphologic aspect (number of channels, channel size distribution, planform sinuosity, shoreline shape). To replicate this complexity we propose a reduced complexity network growth model, based on a set of simple rules some of which are quantitatively anchored in physical processes while others are purely, and connected to the physical process in an implicit way, via observed field correlations among various terms (e.g., Syvitski, 2006). The intent is to keep the number of rules to a minimum necessary to reproduce, in a statistic sense, most but not all of the observed delta styles. In its most general form, the model generates distributary networks in which planform of individual channels emerge from a correlated random walk algorithm, channel density is a function of a prescribed bifurcation probability and the overall delta shape (i.e., wide vs narrow) is controlled through a dependency on dominant flow direction. Individual channels form through successive addition of short segments (piecewise) each new piece introducing a small direction deflection that is partly correlated to the previous deflection. A preferential flow direction (trend) is factored in as a proxy for the downstream slope. The weight assigned to this direction is small but critical in controlling the overall delta shape. This correlated random walk method is equivalent to the one used and tested by Surkan and van Kan (1969). The key to producing networks is channel bifurcation. Frequent bifurcations result in dense, anabranching channel patterns while more representative deltaic networks are obtained using a small probability bifurcation value (0.01 to 0.05). The proposed network growth model can yield distributary networks of significant morphological variation in terms of shapes, channel planforms, or channel density. The comparison between model outcomes and field analogs will be through a series of metrics such as planform shape of individual channels, delta shape, shoreline shape, or channel density distribution. We argue that a stochastic approach driven by simple rules is ideal for investigating complex delta distributaries. Though reduced complexity models employs much simpler rules it does demonstrably lead to complex landscape patterns via randomness built in (e.g. Murray & Paola, 1994). Using simple rules to characterize the process, rather than to model it analytically through complex models, also enables scenario testing and makes it easier to understand the important controls and explore the link between process and landscape.

#### SNAC-CHILD Coupling: Preliminary Results Towards Interoperable Modeling Frameworks

Eunseo Choi, Center for Earthquake Research and Information Memphis Tennessee, United States. echoi2@memphis.edu

Geodynamic modeling of the Earth's subsurface provides critical boundary conditions for surface dynamics and deformation modeling, at various time scales. This in turn may be used to investigate the formation of specific landscape and geology configurations. Linking these two scientific tool chains, and the corresponding communities, through setting up an interoperability protocol between a framework for tectonic modeling applications, Pyre, and the CSDMS model coupling approach is one of the direct aims of the on-going EarthCube Building Blocks project, "Earth System Bridge: Spanning Scientific Communities with Interoperable Modeling Frameworks". I present preliminary works towards coupling SNAC, a Pyre-compatible application for tectonic modeling, with CHILD, a landscape evolution modeling code available as a component of the CSDMS Modeling Toolkit. As a proof of concept, a coupling scheme

has been implemented without making explicit use of any framework. This simplistic coupling scheme is described, validated through non-trivial models, and discussed in terms of the interoperability of frameworks.

#### Challenges in building coastal digital elevation models

Barry Eakins, CIRES Boulder Colorado, United States. <u>barry.eakins@colorado.edu</u> Pamela Grothe, Georgia Institute of Technology Atlanta Georgia, United States.

Digital elevation models support a wide variety of uses, including modeling of surface processes, habitat mapping and conservation planning, coastal change and terrain analysis, and Earth visualization and exploration. These models may, however, contain significant deviations from the surface they are intended to represent, which could reduce their usefulness. Additional complexities arise when integrating bathymetric and topographic data to create coastal DEMs. We identify common challenges in building square-cell, coastal DEMs, and present some solutions. These challenges are grouped into six general categories: (i) source data, (ii) data processing, (iii) model development, (iv) model assessment, (v) morphologic change, and (vi) model uncertainty. Some DEM best practices to help improve DEM accuracy and utility include: visual inspection of source data in a GIS environment; establishing common horizontal and vertical datums; using data buffers and bathymetric pre-surfaces; assessing DEM accuracy; accounting for morphologic change; and quantifying DEM uncertainty at the cell level.

# Modeling sediment-related loading, transport, and inactivation of fecal indicator bacteria at a nonpoint source beach

Zhixuan Feng, University of Miami Miami Florida, United States. <u>zfeng@rsmas.miami.edu</u> Ad Reniers, University of Miami Miami Florida, United States. Brian Haus, University of Miami Miami Florida, United States. Helena Solo-Gabriele, University of Miami Coral Gables Florida, United States.

Enterococci are the U.S. Environmental Protection Agency (EPA) recommended fecal indicator bacteria for assessing recreational marine water quality. Traditional methods of enterococci analyses are time consuming, resulting in delays in issuing beach closures. Models can potentially circumvent these delays by forecasting times when beaches should be closed. The objective of this study is to develop an innovative coupled microbe-hydrodynamic-morphological model. The unique feature of this model is its capability of simulating the release of microbes attached to coastal beach sands as a result of combined wave and tidal forcing. A nearshore process model (XBeach) was coupled with a microbe transport-decay equation. This equation included source functions that accounted for microbial release from mobilized sand, groundwater flow, entrainment through pore water diffusion, rainfall-runoff loading, and a fate function that accounted for solar inactivation effects. The model successfully simulated observed spatial and temporal patterns of enterococci in the beach water, including the reproduction of diel and tidal fluctuations and the rapid decrease of enterococci levels from the waterline to offshore. Primary processes for enterococci loading to the water column included wave-induced sediment resuspension and tidal washing for the entrainment of enterococci from the pore water in the intertidal zone. Diffusion was the major mechanism to transport enterococci from the intertidal zone to offshore. Sunlight inactivation was a key process to reduce enterococci levels during the day and to produce the diurnal cycles. Rainfall runoff was found to be an intermittent source of enterococci to beach water, whereas groundwater exchange was of secondary importance. Sensitivity analyses suggested that the processes and coefficients related to enterococci loading have quasi-linear characteristics, whereas model results of enterococci levels were sensitive to both diffusion and sunlight inactivation coefficients, showing high nonlinearity and spatial and temporal dependence.

#### Modeling the evolution of a thrust system: a geological application of DynEarthSol2D

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DynEarthSol2D (an open source available at http://bitbucket.org/tan2/dynearthSol2) is a robust, adaptive, twodimensional finite element code that solves the momentum and heat energy balance equations in the Lagrangian form using unstructured meshes. Verified in a number of benchmark problems, this solver uses contingent mesh adaptivity in places where shear strain is focused (localization) and a conservative mapping assisted by marker particles to preserve phase boundaries during remeshing. As a first step towards the ultimate goal of applying DynEarthSol2D to the tectonics-surface process coupling, we explored the role of spatial distribution of décollements on structural styles of a thrust system. In our models, a décollement is a gliding zone of accumulated high shear strain, originating from an incompetent layer with a lower cohesion and friction angle than its surrounding rock. Models of various spacing between décollements develop dramatically different subsequent structures with a spectrum of three characteristic styles of thrust systems: ramp-flat thrust, imbricate thrust, and duplex. We also investigate how erosion rates and overburden influence thrusting patterns.

# Changes in water and sediment exchange between the Changjiang River and Poyang Lake under natural and anthropogenic conditions, China

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Jianjun Jia, Key Laboratory of Submarine Geo-Sciences, Second Institute of Oceanography, State Oceanic Administration, Hangzhou, China

Albert J. Kettner, CSDMS Integration Facility, INSTAAR, University of Colorado, Boulder, CO 80309-0545, USA, United States. Fei Xing, CSDMS Integration Facility, INSTAAR, University of Colorado, Boulder, CO 80309-0545, USA, United States.

To study the fluvial interaction between Changjiang River and Poyang Lake, we analyze the observed changes of riverine flux of the mid-upstream of Changjiang River Catchment, Poyang Lake Watershed and Poyang Lake basin. Inter-annual and seasonal variation of the water discharge and sediment exchange processes between Changjiang River and Poyang Lake are systematically explored to determine the influence of climate change as well as human impact (especially the Three Gorge Dam (TGD)). Results indicate that climate variation for the Changjiang catchment and Poyang Lake Watershed is the main factor determining the changes of water exchanges between Changjiang River and Poyang Lake. However, human activities (including the emplacement of the TGD) accelerated this rate of change. Relative to previous years (1956-1989), the water discharge outflow from Poyang Lake during the dry season towards the Changjiang catchment increased by 8.98 km3 y-1 during 2003-2010. Evidently, the water discharge flowing into Poyang Lake during late April-late May decreased. As a consequence, water storage of Poyang Lake significantly reduced during late Aprillate May, resulting in frequent spring droughts after 2003. The freshwater flux of Changjiang River towards Poyang Lake is less during the flood season as well, significantly lowering the magnitude and frequency of the backflow of the Changjiang River during 2003-2010. Human activities, especially the emplacement and operation of the TGD and sand mining at Poyang Lake imposes a major impact on the variation of sediment exchange between Changjiang main river and Poyang Lake. On average, sediments from Changjiang River deposited in Poyang Lake before 2000. After 2000, Changjiang River no longer supplied sediment to Poyang Lake. As a consequence, the sediment load of Changjiang River entering the sea increasingly exists of sediments from Lake Poyang during 2003-2010. As a result, Poyang Lake converted from a depositional to an erosional system, with a gross sediment loss of 120.19 Mt y-1 during 2001-2010, including sand mining.

### An iterative bleach-and-mix model for the change in luminescence signal with cumulative sediment transport. Harrison Gray, University of Colorado – Boulder, *Colorado, United States* <u>harrison.gray@colorado.edu</u>

Optically Stimulated Luminescence (OSL) dating is one member of a family of dating techniques that rely on sufficient sunlight exposure (bleaching) to remove a previously obtained signal. Sunlight exposure occurs during sediment transport from original erosional source to depositional sink and the presence of this signal bleaching is well-documented in the literature, yet, the mechanics of sunlight exposure in geomorphic systems has been unexplored. Since this bleaching of luminescence signal is a function of geomorphic variables such as transport rate, mechanism, and sediment flux, there exists potential to quantify these processes through measurement of the luminescence signal at various locations within a geomorphic system.

Here, I present a simple model demonstrating the predicted change in luminescence signal for a package of sediment with a homogeneous initial signal that is iteratively bleached at the surface and re-mixed. The model does not attempt to directly model a specific geomorphic environment, but is a starting point for predicting the magnitude and dispersion of luminescence signal values throughout a geomorphic system. Initial model results demonstrate that the mean luminescence signal should decrease in a power law fashion asymptotically approaching zero with each mixing event. The standard deviation of the sediment package increases rapidly during the early mix and bleach iterations before leveling off and decreasing toward zero as the majority of the sediment reaches a homogeneously bleached state. Introducing a sediment flux into and out of the sediment package alters the geometry of the package and therefore the efficiency of bleaching causing the mean and standard deviation to approach steady-state values. This may suggest that the luminescence signals measured from sediment in transport act as a proxy for volumetric sediment fluxes. Combining this model with landscape evolution models may help predict the luminescence signal for fluvial networks which may in turn assist in provenance studies.

# Measuring the imprint of orographic rainfall gradients on the morphology of steady-state numerical landscapes

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In this study we incorporate a 2-D orographic precipitation module into the CHILD numerical landscape evolution model to provide a quantitative tool for exploring the coevolution of rainfall patterns and fluvial topography, focusing on the imprint of spatial rainfall patterns on steady-state landscapes with uniform rock uplift. Our results suggest that network organization and planform morphology are strongly impacted by rainfall patterns. We find that rainfall gradients produce narrower watersheds, because channels show a tendency to flow along the rainfall gradient, rather than across it. The change in watershed shape is evidenced by smaller values of the exponent on distance in Hack's law and a less peaked width function, which describes the distribution of points in a network at a given length from the outlet. Narrower watersheds also lead to an increase in the valley spacing ratio (mean mountain half width over mean distance between adjacent mainstem river outlets) and constrain trunk channels to follow a more direct path to the mountain foot. Rainfall gradients also influence the distribution of topography across a watershed. Channel profiles record rainfall patterns in both the channel concavity (downstream changes in slope) and the channel steepness index (ksn, or local slope normalized for drainage area). Small tributaries, in which the rainfall rate does not change as much relative to the mainstem channels, have a relatively clear relationship between ksn and mean rainfall across the tributary watershed. The hypsometric integral (HI), which increases with the amount of topography that is at relatively high elevations within a watershed, has a negative relationship with the profile concavity of the trunk channel, and high rainfall rates at the ridge top lead to mainstem channels that have relatively low concavity and watersheds with relatively higher HI in comparison with landscapes that have uniform precipitation. We contrast the impacts of rainfall patterns on landscape morphology with those resulting from a linear uplift gradient and uniform rainfall. We find that uplift patterns may have a similar impact on landscape morphology as rainfall gradients, making it challenging to decipher the relative roles of climate and tectonics on landscape evolution.

# Tidal Modulated Flow and Sediment Flux through Wax Lake Delta Distributary Channels: Implications for Delta Development

Kevin Hanegan, University of New Orleans New Orleans Louisiana, United States. <u>khanegan@uno.edu</u> Ioannis Georgiou, University of New Orleans New Orleans Louisiana, United States. <u>igeorgio@uno.edu</u>

In this study, a Delft3D model of the Wax Lake Delta was developed to simulate flow and sediment flux through delta distributary channels. The model was calibrated using existing measurements of velocity and sediment concentration across channel transects taken during a single flood event. The calibrated model was then used to simulate full springneap tidal cycles with several representative upstream boundary conditions, with grain size variation in suspended load represented using two sediment fractions. Flow and sediment flux results through distributary channel cross-sections

were examined for spatial and temporal variability with the goal of characterizing delta development processes at the scale of a single bifurcation and along the entire channel network. The Wax Lake Delta has grown through channel extension, mid-channel bar deposition, and channel bifurcation. The formation of stable bifurcations in the delta has controlled the resulting channel network and landscape development. Model results at two particular bifurcations with varying degrees of asymmetry are examined in light of proposed equilibrium conditions. The flow and sediment flux distributions at both bifurcations show variability through the tidal cycle and at different input discharges. Additionally, the trends in flow, velocity, bed shear stress, and sediment transport are examined along primary distributary channels. Here we show that tidal modulation of currents influences suspended sand transport, and ebb-tide acceleration has the capacity to suspend sand in distal reaches during lower flows. The basinward-increasing transport capacity in Wax Lake Delta channels indicates that erosive channel extension could be an important process even during non-flood events. Results of this study show that tidal range and varying flow influence the balance between erosional and depositional delta growth. Modeling of these processes in existing deltas can increase the understanding of dynamics during low-flow portions of the year and their importance in delta development.

# Interrogating the Sensitivity of Snow-Season Water and Energy Fluxes from a Land-Surface Model to High-Resolution Forest Canopy Information

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Snowmelt from forested areas is critical to the management of ecosystem services and water resources in the Western U.S. Current land-surface models use relatively simple forest canopy parameterizations that neglect spatial. Highresolution forest canopy information collected using Light Detection and Ranging (LiDAR) has the potential to inform these models and increase the model fidelity of snow-vegetation interactions. In this study, we apply the Noah-MP (multi-parameterization) land-surface model to ask the study question "How does higher resolution parameterizations of forest canopy structure in a land-surface model alter the timing and magnitude of snow-season water and energy fluxes across a variety of Western U.S. mixed-conifer forests?". To answer this question we developed tree geometry (height and radius), stem density, and canopy cover parameters from LiDAR for a 2 by 2 km area at scales of 1, 0.5, and 0.1 km at four sites: Boulder Creek, CO, Jemez, NM, Kings River, CA, and Wolverton, CA. We ran the Noah-MP model at these scales using the Niwot Ridge, CO Ameriflux forcing to investigate model response to a wet (2011) and dry (2012) year. The model resolution produced noticeable differences in the timing of snowmelt at all sites, with the 0.1 km model having earlier and larger snow ablation due to greater turbulent heat fluxes from model grid cells having little to no forest cover. The higher resolution model also produced greater longwave radiation losses to the atmosphere. Compared to snow water equivalent (SWE) observations near Niwot Ridge, the coarser models (0.5 and 1 km) tended to accumulate too much snowpack and melt snow too rapidly, while the finer resolution model (0.1 km) tended to ablate too much snow mid-winter but captured the timing of peak SWE and snowmelt more robustly. The forest canopies from the four different sites did little to alter the timing of snow accumulation and ablation at the coarser resolutions. Interestingly, the 0.1 km model showed characteristic accumulation and ablation timing at each of the four sites that were consistent with their different forest canopies. Our results suggest that higher resolution Noah-MP model runs resulted in water and energy fluxes that were generally more consistent with a variety of in-situ observations. However, land-surface models may need to adjust their turbulent transfer parameters and/or share information on turbulent heat fluxes between model grid cells in order to fully utilize high resolution forest canopy information.

#### InSAR measurements of compaction and subsidence in the Ganges-Brahmaputra Delta, Bangladesh

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The Ganges-Brahmaputra Delta (GBD) is the world's largest river delta, and is home to more than 150 million people. This study reconstructs subsidence rates in the eastern portion of the Ganges-Brahmaputra Delta (GBD), Bangladesh, covering more than 10,000 km2 at a high spatial resolution of 100 m. The map was produced using Interferometric Synthetic Aperture Radar (InSAR) covering the period 2007 to 2011. Eighteen ALOS (Advanced Land Observing Satellite) PALSAR (Phased-Array L-band SAR) scenes were used to generate 30 interferograms calibrated with GPS. Interferograms were stacked to yield average subsidence rates over the study period. Small Baseline Subset (SBAS)-

InSAR was then applied to validate the results against an additional GPS record from Dhaka, Bangladesh. Land subsidence of 0 to > 10 mm/y is seen in Dhaka, likely related to groundwater abstraction with rates corresponding to local variations in shallow subsurface sediment properties. Outside of the city, rates vary from 0 to > 18 mm/y, with the lowest rates appearing primarily in Pleistocene Madhupur Clay and the highest rates in Holocene organic-rich muds. Results demonstrate that subsidence in this delta is primarily controlled by local stratigraphy, with rates varying by more than an order of magnitude depending on lithology. The ability of L-band InSAR to differentiate between stratigraphic units in this humid, vegetated subtropical river delta demonstrates the power of interferometry as a tool for studying the subsurface in deltaic environments.

#### Exploring how parameter importance to prediction changes in parameter space

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This talk presents a novel hybrid local-global method that measures how model parameter importance is distributed as parameter values change. DELSA (Distributed Evaluation of Local Sensitivity Analysis) is demonstrated using rainfallrunoff models constricted using FUSE, and results are compared to the Sobol' global sensitivity analysis method. Insights from DELSA can be combined with field data to identify the most relevant parts of parameter space to focus data collection and model development. Much of what will be discussed is described in: Rakovec, O., M. C. Hill, M. P. Clark, A. H. Weerts, A. J. Teuling, and R. Uijlenhoet (2014), Distributed Evaluation of Local Sensitivity Analysis (DELSA), with application to hydrologic models, Water Resources Research, 50, doi:10.1002/2013WR014063.

# Understanding wave-driven fine sediment transport through 3D turbulence resolving simulations – implications to offshore delivery of fine sediment

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One of the most intriguing issues in fine sediment transport, including turbidity currents, current-driven transport and wave-driven transport, is that the presence of sediments may significantly attenuate flow turbulence. Depending on the level of turbulence suppression, it may lead to the formation of lutocline (a sharp negative gradient of sediment concentration) which further encourages offshore-directed gravity flow; or it may cause catastrophic collapse of turbulence and sediment deposition. Through idealized 3D turbulence-resolving simulations of fine sediment (mud) transport in wave bottom boundary layer based on a pseudo-spectral scheme, our recent studies show that the transition of these flow modes can be caused by various degree of sediment-induced stable density stratification. This effort demonstrates the success of using a turbulence-resolving simulation tool to diagnose complex fine sediment transport processes. This talk further reports our recent development of this turbulence-resolving numerical model with a goal to provide a predictive tool for more realistic fine sediment transport applications. Assuming a small Stokes number (St<0.3), which is appropriate for typical fine sediment, the Equilibrium approximation to the Eulerian two-phase flow equations is applied. The resulting simplified equations are solved with a high-accuracy hybrid spectral-compact finite difference scheme. The numerical approach extends the earlier pseudo-spectral model with a sixth-order compact finite difference scheme in the bed-normal direction. The compact finite difference scheme allows easy implementation of flow-dependent sediment properties and complex bottom boundary conditions. Hence, several new capabilities are included in the numerical simulation, such as rheological stress (enhance viscosity in high sediment concentration), hindered settling, erodible/depositional bottom boundary, and higher order inertia terms critical for fine sand fraction. In the past decade, the role of wave bottom boundary layer in delivering fine sediment offshore via wave-supported gravity current (WSGC) has been well-recognized. We hypothesize that the generation, transport and termination of WSGC is directly associated with the flow modes discussed previously. In addition to the well-known Richardson number control (i.e., associated with sediment-induced density stratification), in this talk we will discuss how enhanced viscosity via rheological stress and high erodibility of the mud bed (e.g., low critical shear stress for unconsolidated mud bed) can trigger catastrophic collapse of turbulence and sediment deposition. The significance of bed erodibility in determining the resulting flow modes motivates future study regarding the effect of sand fraction on fine sediment transport via armoring.

#### Using ground-penetrating radar to measure an ice-wedge depth

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We use 2-D forward finite-difference model of the ground-penetrating radar (GPR) to recover ice-wedge depth. The results of the inverse modeling of the synthetic ice-wedge depth showed convergence to the prescribed values. Here we present preliminary results of the synthetic ice-wedge depth recovery using genetic algorithm optimization subroutine. We also applied some noise to the synthetic data and showed up to what level of noise we were able to recover the desired depth. To evaluate the inverse method we calculate the corresponding uncertainties.

#### Advances in sediment transport modeling offshore of a fluvial source

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The Community Sediment Transport Modeling System (CSTMS) has been applied to several continental shelf environments, including areas offshore of large river sources. However, all of these sediment transport model studies have represented sediment as non-reactive tracers, resulting in a disconnection between model calculations and field observations which may rely on geochronological tracers. Additionally, model estimates of sediment transport within the freshwater plume, or resuspended on the sediment bed have not been linked to cross-shelf transport mechanisms that carry material to the deep sea. Here we make advances on both fronts by developing a numerical model for suspended transport that will be linked to models of down-slope transport, and furthermore develop the ability to directly estimate transport and decay of particle reactive radionuclides. To better understand transport pathways and depositional patterns in the Gulf of Mexico, a three-dimensional coupled hydrodynamic-sediment transport model has been developed within the Regional Ocean Modeling System (ROMS). The modeled period, October 2007 through September 2008, included two hurricanes and a period of high river discharge. Model estimates of sediment dispersal revealed sensitivities to settling velocities and critical bed shear stresses. Transport and deposition of terrestrial sediments were limited alongshelf, such that the model showed little comingling of material from the Mississippi, Atchafalaya, and Mobile Rivers during the yearlong model run. Across-shelf suspended sediment transport occurred primarily during periods of elevated wave heights, coincident with storms. The relative influences of terrestrial and marine processes on sediments in coastal marine environments can be inferred from the distribution of short-lived radioisotopes, but these have not previously been represented within models. A one-dimensional (vertical) sediment transport model was modified to include Be-7, a proxy for terrestrial sources, and Th-234, a proxy for suspension in marine environments, as reactive tracers associated with sediment particles. Experimental results explored the sensitivity of vertical radioisotope profiles to initial deposit thickness, bioturbation rates, resuspension depths, and initial radioisotope inventories. This approach will facilitate better comparisons between modeled and observed sediment transport and depositional data.

#### Spatial structure and evolution in emergent vegetated ecosystems

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Predicting how plant-water landscapes evolve through time is essential for development and restoration work involving natural ecosystems and built environments near waterways. Recent experimental studies show that the interaction and merger of vegetation patch wakes can produce zones of diminished velocity and enhanced deposition that persist downstream and are offset from the patch centerline, which may encourage lateral patterns of growth. These effects are not incorporated into current models of landscape evolution. In this study, these flow-biogeomorphic interactions at the patch scale are incorporated into a simple model for vegetation development. The model is constructed in Matlab, utilizing MODFLOW, based on a porous media formulation for hydraulic resistance. Landscape evolution over 5 to 300 cycles of vegetation growth produces several categories of realistic landforms. The effect of wakes is shown to

consistently alter the steady-state landscape reached by an environment, implying that current models underestimate the effects of vegetation on development.

#### Unifying Tectonics and Surface Processes in Geodynamics

#### Peter Koons, University of Maine

In formulating tectono-geomorphic models of landscape evolution, Earth is typically divided into two domains; the surface domain in which "geomorphic" processes are solved for and a tectonic domain of earth deformation driven generally by differential plate movements. Here we present a single mechanical framework, Failure Earth Response Model (FERM), that unifies the physical description of dynamics within and between the two domains. FERM is constructed on the two, basic assumptions about the three-dimensional stress state and rheological memory: I) Material displacement, whether tectonic or geomorphic in origin, at or below Earth's surface, is driven by local forces overcoming local resistance, and II) Large displacements, whether tectonic or geomorphic in origin, irreversibly alter Earth material properties enhancing a long term strain memory mapped into the topography. In addition to the gathering of stresses arising from far field tectonic processes, topographic relief, and the inertial surface processes into a single stress state for every point, the FERM formulation allows explicit consideration of the contributions to the evolving landscape of pore pressure fluctuations, seismic accelerations, and fault damage. Incorporation of these in the FERM model significantly influences the tempo of landscape evolution and leads to highly heterogeneous and anisotropic stress and strength patterns, largely predictable from knowledge of mantle kinematics. The resulting unified description permits exploration of surface-tectonic interactions from outcrop to orogen scales and allows elucidation of the high fidelity orogenic strain and climate memory contained in topography.

#### Developing and evaluating algorithms for lateral erosion of bedrock channels in landscape evolution models

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Theory for the vertical incision of bedrock channels is well established and is widely implemented in our current generation of landscape evolution models. However, existing models in general do not seek to implement rules for lateral migration of bedrock channel walls. This is problematic, as geomorphic problems such as terrace formation and hillslope-channel coupling depend heavily on accurate simulation of valley widening. We have begun to develop and implement a theory to represent the lateral migration of bedrock channel walls in a landscape evolution model. In a real channel, rates of lateral channel wall erosion depend on the shear stress directed at the channel walls and the resisting strength of the bedrock. Shear stress directed at the channel walls is a function of channel curvature, discharge magnitude, and sediment supply, which provides tools to abrade the walls and cover to shield the bed from erosion. We used previously published experimental data showing the influence of sediment flux and discharge on bedrock channel incision to determine the amount of lateral erosion based on a relationship between sediment flux and discharge. These data indicate a relationship between increasing sediment flux and bed cover and increasing lateral erosion. We use the Landlab modeling environment to abstract these rules for lateral erosion of channel walls to a landscape evolution model. Our model algorithm calculates total erosion rate at each cell and then partitions that erosion into vertical or lateral erosion. The amount of lateral erosion is calculated using Qs/Qt, the ratio of total sediment flux at a cell to total transport capacity. The vertical erosion is applied to the primary cell, while the lateral erosion component is applied to a neighboring cell chosen at random, allowing the stream network to shift when the elevation in the neighboring cell becomes lower than that of the primary cell. These simple rules for including lateral erosion in a gridded model result in wider valleys and more dynamic stream networks, especially in landscapes with weak bedrock. In particular, the model simulates erosive fluvial valley floors that are more than a grid cell wide, maintains them in the face of continuing landscape uplift, and creates terraces in the landscape in response to varying sediment supply to the channels. To our knowledge, these efforts represent the first attempt to incorporate lateral erosion in a network-based landscape evolution model.

# Towards better quantifications of the uncertainty in polar ice-sheet projections using the open source framework ISSM

Eric Larour, Jet Propulsion Laboratory

Understanding and modeling the evolution of continental ice sheets such as Antarctica and Greenland can be a difficult task because a lot of the inputs used in transient ice flow models, either inferred from satellite or in-situ observations, carry large measurement errors that will propagate forward and impact projection assessments. Here, we aim at comprehensively quantifying error margins on model diagnostics such as mass outflux at the grounding line, maximum surface velocity and overall ice-sheet volume, applied to major outlet glaciers in Antarctica and Greenland. Our analysis relies on uncertainty quantification methods implemented in the Ice Sheet System Model (ISSM), developed at the Jet Propulsion Laboratory in collaboration with the University of California at Irvine. We focus in particular on sensitivity analysis to try and understand the local influence of specific inputs on model results, and sampling analysis to quantify error margins on model diagnostics. Our results demonstrate the expected influence of measurement errors in surface altimetry, bedrock position and basal friction.

#### A vector-based method for bank-material tracking in coupled models of meandering and landscape evolution Ajay Limaye, *California Institute of Technology*

Sinuous channels commonly migrate laterally and interact with banks of different strengths—an interplay that links geomorphology and life, and shapes diverse landscapes from the seafloor to planetary surfaces. To investigate feedbacks between meandering rivers and landscapes over geomorphic timescales, numerical models typically represent bank properties using structured or unstructured grids. Grid-based models, however, implicitly include unintended thresholds for bank migration that can control simulated landscape evolution. I will present a vector-based approach to land surface- and subsurface-material tracking that overcomes the resolution-dependence inherent in grid-based techniques by allowing high-fidelity representation of bank-material properties for curvilinear banks and low channel lateral migration rates. The vector-based technique is flexible for tracking evolving topography and stratigraphy to different environments, including aggrading floodplains and mixed bedrock-alluvial river valleys. Because of its geometric flexibility, the vector-based material tracking approach provides new opportunities for exploring the co-evolution of meandering rivers and surrounding landscapes over geologic timescales.

#### The Dynamics of Granular Flows

#### Jim McElwaine, Durham University (UK)

Granular materials are ubiquitous in the environment, in industry and in everyday life and yet are poorly understood. Modelling the behavior of a granular medium is critical to understanding problems ranging from hazardous landslides and avalanches in the Geosciences, to the design of industrial equipment. Typical granular systems contain millions of particles, but the underlying equations governing that collective motion are as yet unknown. The search for a theory of granular matter is a fundamental problems in physics and engineering and of immense practical importance for mitigating the risk of geohazards. Direct simulation of granular systems using the Discrete Element Method is a powerful tool for developing theories and modelling granular systems. I will describe the simulation technique and show its application to a diverse range of flows.

# Sediment Dynamics of the Lower Mississippi River: Understanding Sediment Availability and Delivery for Land Building

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There is a dire need to use sediment from alluvial rivers to sustain and create new marsh, sustain barrier islands and ridges. Coastal Louisiana is a prime example where wetland loss rates are one of the highest worldwide. This presentation discusses the sediment dynamics of the Lower Mississippi River, specifically the sediment availability, temporal and spatial variability, as well as the sediment size characteristics. The investigation is performed using morphodynamic numerical tool (Delft3D). The Louisiana 2012 State Master Plan identified two viable mechanisms to build land, sediment diversions and dedicated dredging. The morphodynamic model has been parameterized and validated using historical and recent field observations. The model is being used to investigate the riverside morphological response to single or multiple dredging of lateral sand bars as well as the infilling pattern and rate. The

model will also be used to identify the key design parameters that govern the sediment capture efficiency of sediment diversions, e.g. the alignment angle, invert elevation, diversion size, and location.

The uncertainty and limitations in the ability of the numerical model to adequately capture the relevant physical processes is discussed. The implications of such limitations on the decision making process is presented. Despite the limitations and uncertainties, the analysis provides valuable design recommendation for sediment diversions to maximize their sediment capture efficiency. The analysis also provides a management plan for dredging multiple borrow areas. The management plan includes coordination of dredging timeline among multiple borrow pits, as well as coordination between dredging activities and sediment diversion operation plans.

#### Including sediment patches in sediment transport predictions in steep mountain channels

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Spatial variability in grain size, roughness and sorting generated by bed surface patches impact bedload transport by altering the relative local mobility of different grain sizes and creating complex local flow fields. In high gradient mountain channels large roughness elements bear a significant portion of the total shear stress available for motion and the remaining shear stress acts over patches of more mobile sediment. The shear stress on mobile patches has a distribution of values that depend on the local topography, patch type, and location relative to roughness elements and the thalweg. Current sediment transport equations do not account for these variations of roughness, local flow, and grain size distributions on and between patches. Often they use an area-weighted approach to obtain a representative grain size distribution and reach-averaged shear stress and by doing so they lose important characteristics that affect sediment transport estimations. Such equations also do not distinguish between active (patches where at least one grain size is in motion) and inactive patches and do not include differences in mobility between patch classes that results from local hiding effects and spatial shear stress distributions. We hypothesize that predictions of sediment transport must explicitly include different patch classes and local variations of the flow field. We modified Parker's (1990) bedload transport equations to use distributions of shear stresses, measured grain sizes, and a specific hiding function for each patch class. A reach averaged sediment transport rate was calculated considering the contributions of all the different patch classes. To test this hypothesis we calculated the distributions of shear stresses over a range of patch classes in a 40 m long, 10% gradient step-pool stream. We surveyed the bed with a high density resolution (5 cm in horizontal and vertical), mapped and classified patches by their grain size distributions, and measured water surface elevations and mean velocities for low to moderate flow events. With these data, using a quasi-three dimensional model (FaSTMECH), shear stress distributions were calculated over each patch for a range of flow discharges. Shear stress distributions varied between different patch classes and also changed for different discharges. Sediment mobility in patches was highly dependent on the patch's class and location relative to the thalweg and large roughness elements. Predicted bedload transport rates more closely matched measured values when patch classes instead of individual patches were used. More accurate bedload predictions were obtained if the shear stress distribution shape was allowed to change with discharge. Compared to deterministic formulations, the use of distributions of shear stress and bed grain sizes significantly improved predictions of bedload transport in a steep mountain channel.

#### Buoyant and Gravity-Driven Transport on the Waipaoa Shelf: Model Evaluation and Sensitivity Analyses

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Riverine deposits on continental shelves display terrestrial signatures, although the marine environment may overprint them. Partitioning between various transport mechanisms (dilute suspension vs. gravity-driven) may influence the location and characteristics of these deposits. The MARGINS Waipaoa River shelf initiative investigated these issues by conducting a thirteen month field campaign, and an ongoing numerical modeling study of the Waipaoa River shelf, New

Zealand. We used two numerical models to analyze sediment fluxes and fate on the continental shelf during a time when three large floods and multiple high wave events occurred, from January 15, 2010 – February 15, 2011.

Water-column fluxes were estimated using the Regional Ocean Modeling System- Community Sediment Transport Modeling System (ROMS - CSTMS). This three-dimensional hydrodynamic-sediment transport numerical model accounted for gravity-driven transport by incorporating sediment concentrations into the model's equation of state. Because ROMS did not resolve fluxes within the thin wave-current boundary layer, however, we also used a linear-bed turbid layer model based on the Chezy equation, which balances friction and gravity. Buoyant fluxes within the water column model distributed sediment along-shore to the inner and mid-shelf, depositing material up to about 50 m water depth. Wave- and current- supported gravity flows, in contrast, could export sediment to long-term shelf depocenters (50 - 70 m water depth) and the continental slope. Hydrodynamic and seabed observations of sediment fluxes and gravity flows will be compared to sensitivity tests. Preliminary results indicated that erodibility parameterization and sediment settling velocity significantly affected buoyant sediment fluxes. In contrast, estimates from the near-bed turbid layer model were sensitive to assumptions about the distribution of sediment delivery from the river in terms of the initial deposit and percentage of the riverine load available for gravity driven transport.

#### Modelling the evolution of large river floodplains

Andrew Nicholas, University of Exeter

Floodplain construction involves the interplay between channel belt sedimentation and avulsion, overbank deposition of fines, and sediment reworking by channel migration. There has been considerable progress in numerical modelling of these processes over the past few years, for example, by using high resolution flow and sediment transport models to simulate river morphodynamics, albeit over relatively small time and space scales. Such spatially-distributed hydrodynamic models are also regularly used to simulate floodplain inundation and overbank sedimentation during individual floods. However, most existing models of long-term floodplain construction and alluvial architecture do not account for flood hydraulics explicitly. Instead, floodplain sedimentation is typically modelled as an exponential function of distance from the river, and avulsion thresholds are defined using topographic indices (e.g., lateral:downstream slope ratios or metrics of channel belt super-elevation). This presentation aims to provide an overview of these issues, and present results from a hydrodynamically-driven model of long-term floodplain evolution. This model combines a simple network-based model of channel migration with a 2D grid-based model of flood hydrodynamics and overbank sedimentation. The latter involves a finite volume solution of the shallow water equations and an advection-diffusion model for suspended sediment transport. Simulation results are compared with observations from several large lowland floodplains, and the model is used to explore hydrodynamic controls on long-term floodplain evolution and alluvial ridge construction.

#### Wave angle control on deltaic channel orientation

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Deltas are fragile coastal ecosystems, sensitive to changes in both marine and terrestrial forcings. Many active deltas face rising sea level, reduced fluvial sediment supply, and a subsiding delta plain, making them increasingly exposed to wave action. In a deltaic system, autogenic feedbacks between the river mouth, alongshore transport of sediment, and differential morphology between the up and downdrift flanks of the delta can deflect the river mouth and steer the course of the river. Previous modeling studies of wave-influenced deltas forced the fluvial channel to grow along a straight, predefined path, leaving these feedbacks unexplored. We improve upon the plan-view delta Coastline Evolution Model (CEM) by allowing the river mouth to grow in a direction perpendicular to the local shoreline's orientation. Additionally, a fraction of littoral sediment  $\beta$  can bypass the river mouth. This allows us study the effects of wave climate and sediment bypassing on channel orientation. We find that for a large fluvial sediment flux the channel will orient itself into the dominant wave approach direction. In this case, shoreline angles on both sides of the river mouth effectively limit sediment bypassing. As fluvial dominance decreases, the channel steers away from the waves. When no littoral sediment is allowed to bypass the river mouth, the ratio between the flux of alongshore littoral sediment (stored

in the updrift flank) and the flux of fluvial sediment (stored in the downdrift flank) is reflected by the average channel orientation. This physical framework allows us to further interpret the conditions under which deltas form. Furthermore, these results provide quantitative insight into active deltas under dynamic environmental conditions.

#### Coupling Fluvial and Eco-hydrologic Components in the Landlab Modeling Framework

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In arid and semi-arid regions, geomorphic response of a catchment is tightly coupled with Eco-hydrologic dynamics. Climate-driven biotic and abiotic processes strongly influence land-surface-atmosphere interactions and thus play an important role in landscape evolution. Landscape Evolution Models (LEMs) provide a platform for scientists to quantitatively understand these complex interactions by exploring testable hypotheses. Hydrology and vegetation dynamics are thus critical components of these LEMs. This work illustrates the development of such components and model-building by coupling fluvial and ecohydrologic components in the Landlab modeling environment. The Landlab is a component based framework for 2D numerical modeling, coded in Python. It provides a gridding module and allows users to either configure a model from scratch or use existing components. We present a coupled overland flow and vegetation dynamics model where vegetation is simulated based on inputs from stochastic precipitation generator, radiation component, potential evapotranspiration component and soil moisture component, and runoff is routed by overland flow component. This work demonstrates the flexibility of the Landlab and also highlights the advantages of component-based approach.

#### The long-term evolution of normal faults controlled by lithospheric flexure and surface processes

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We investigate the growth of normal faults on long timescales (10-1000 kyrs) and seek to identify key mechanical controls on fault dip, lifespan, and related topography. To do so, we consider the energy budget of a growing fault, which is partitioned into 1/ overcoming the frictional resistance on the fault and 2/ sustaining the build-up of topography and associated flexure. Our model builds on classic finite extension theory, but incorporates the possibility that the active fault plane may rotate as a response to the accumulation of flexural stresses with increasing extension. We postulate that fault plane rotation acts to minimize the amount of extensional work required to keep the fault active. In an elastic layer, this assumption results in rapid rotation of the active fault plane from ~60° down to 30–40° before fault heave has reached 40% of the faulted layer thickness. In our model, fault rotation rates scale as the inverse of the faulted layer thickness, which is in quantitative agreement with 2D geodynamic simulations that include an elasto-plastic description of the lithosphere. We show that fault rotation promotes longer-lived fault extension compared to continued slip on a high angle normal fault, and therefore holds a strong control on faulting styles (i.e., multiple short-offset vs. dominant large-offset faults). Finally, we incorporate erosion and deposition processes into the model, which locally enhance or relieve a portion of the topographic load, and characterize their influence on the evolution of extensional systems.

#### Predicting the influence of floodplain vegetation on the geomorphic effects of large floods Mariela Perignon, University of Colorado

The spatial distribution of vegetation along the banks and floodplains of a river can drastically affect its geomorphic response to large floods. Plants influence sediment transport dynamics and the resulting patterns of erosion and deposition by steering the flow, changing the scale and intensity of turbulence, and increasing the effective cohesiveness

of surface material. Efficiently simulating these interactions over river reaches requires simplifying the small-scale processes into measurable parameters that can reproduce the large-scale behavior of the system.

We present simulations of the evolution of the morphology of vegetated, mobile sand-bed rivers during this flows that were obtained by coupling the existing hydrodynamic model ANUGA with modules for sediment transport and vegetation. This model captures the effects of vegetation on mean flow velocity by treating plant stems as cylinders of specified diameter and spacing and calculating the drag they impart on the flow. The outputs of this model were tested against a well-constrained natural experiment to determine the accuracy of the model predictions. Multi-temporal airborne lidar datasets capture the topographic change that occurred along a 12-km reach of the Rio Puerco, New Mexico, as a result of a large flood in 2006. The magnitude of deposition on the floodplain was found to correlate with vegetation density as well as distance from the primary sediment source. This relationship is reproduced by the model using only the simplest drag formulation. The local variability in deposit thickness was seen to depend strongly on the dominant species present, suggesting that plant-scale processes are reflected in the patch-scale behavior of the system. This indicates a need for more complex parameters that reflect the changes in turbulent energy and shear stress that result from different plant characteristics.

# Testing the efficacy and uncertainty of outcrop- and model-based studies through collaboration: A field geologist's perspective

#### David Pyles, Chevron Center of Research Excellence, Colorado School of Mines

Recent technological advances in data collection techniques have yielded opportunities to better quantify stratigraphic stacking patterns, flow processes and sedimentation from outcrops of ancient sediment transport systems. These advancements created opportunities for field geologists to reduce uncertainty in the interpretation of the stratigraphic record and have likewise created data sets from which the efficacy of numerical models and physical experiments can be evaluated. The goals of this presentation are to (1) review some combined outcrop-model based studies, (2) discuss how these integrated studies test model and field-based uncertainty, and (3) share a vision for how field geologists and modelers can leverage from each other's perspectives.

Five examples of studies that bridged the gap between outcrop stratigraphy and experimental and/or numerical models include: (1) documentation of how mineralogy varies spatially in submarine fans, (2) relating flow processes to sedimentation in sinuous submarine channels, (3) evaluating compensational stacking in deltas and submarine fans, (4) relating stratigraphic architecture of deltas to inherited water depth and seafloor gradient, and (5) testing how shelf-edge deltas pipe coarse-grained sediment to submarine fans. These and similarly focused studies are important because they used common workflows and quantitative methods to evaluate similarities and differences between modeled and natural systems, resulting in a more complete view of the processes and products being studied. Whereas common workflows can provide a means to test the efficacy of physical and numerical modeling, it is critical to consider how modeling sheds insight into how one interprets the stratigraphic record from outcrop and subsurface data sets.

#### Parameter Optimization for a Headcut Erosion Model

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In order to understand the geomorphic legacy of headcut retreat, we have developed a numerical model that simulates headcut erosion over time. One of the difficulties with this type of modeling is the uncertainty in the model parameters. For example, there is limited data for estimates of the resistive shear stress of a grassy channel. Moreover, some parameters, such as soil infiltration capacity, vary in space, and in-situ field measurements can overestimate the actual infiltration that occurs during rainfall events at the watershed-scale. Traditional optimization techniques are not an option because our model is non-differentiable. Consequently, we estimate the best-fit parameters for the model by using a parallel evolutionary algorithm on a cluster supercomputer. Our model uses conservation of mass for both water and sediment to predict how overland flow erosion and deposition, combined with headcut retreat, will shape the longitudinal profile of a channel over time. We simulate channels that are mostly grass-lined, and thus take into consideration the roughness changes in grassy areas and the changes in erodibility. Within the model we optimize ten independent variables, including the critical shear stress for erosion, channel roughness, and effective site infiltration.

The Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is an iterative process where samples are created based on a distribution of parameter values that evolves over time to better fit the features of the objective function. We use this algorithm to optimize the parameters of our model. Initially the distribution will explore more of the parameter space. As the CMA-ES iterates, the distribution changes in size and shape to focus the samples in a region of the parameter space that is more likely to have effective solutions. CMA-ES is able to efficiently find effective parameters, even with high dimensional objective functions that are non-convex, multimodal, and non-separable. We ran model instances in parallel on a high-performance cluster supercomputer, and from hundreds of model runs we obtained the best parameter choice. Initial results of best-fit model parameters were obtained by CMA-ES without requiring a timeintensive, brute force combinatorial approach to explore a 10 dimensional parameter space. This effort revealed a convergence of certain parameters toward a single value, such as the critical basal shear stress. However, some pairs of parameter values diverged (for example, precipitation and infiltration rates) show up to four values that produced similar results. The non-convergence of some parameter values is useful in showing that some physical processes are nonunique, but can still produce a similar morphology. CMA-ES pinpoints these non-unique areas, which allows for further investigation of the physical reality and sensitivity of parameter choices. This offers increased efficiency compared to the testing of every single parameter choice. In summary, this study is a proof of concept for employing advances in computer science optimization to a numerical model simulating geomorphic processes. We are thus able to solve the problem of parameter choice for variables that are difficult or impossible to measure by using an objective methodology. It is likely that many models in the earth science community would benefit from this type of analysis.

#### Simplifying the Ganges-Brahmaputra sediment dispersal system using a coupled model-field approach

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The Ganges-Brahmaputra (G-B) Delta is a densely populated (~900 km-2) delta that could be flooded within the next century by a combination of global sea level rise and increased monsoonal rains. These rivers currently transport a combined estimate of one billion tons of sediment from their basins in the Himalaya Mountains to the delta surface each year during the five months of the Asian summer monsoon. Sediment and water discharge has been reconstructed using observational data from two gauging stations on the Ganges and Brahmaputra Rivers from the mid 1950's onward. However, downstream spatial distribution of sediment flux into the deltaic distributary channel network and deposition rates onto the floodplain and lower deltaplain are remarkably unconstrained, yet critical to understanding the overall delta sediment budget. A series of model components are used to simplify the G-B sediment routing system and to test the sensitivity of the system to various climate scenarios. We numerically model daily and monthly incoming sediment flux with the climate-driven hydrological model, HydroTrend, which predicts long-term sediment load as a function of river discharge, drainage basin characteristics and climate controls. The estimated flux provides boundary conditions to the lowland sedimentary input system. We then present a simple approach to sediment routing over the delta distributaries and into tidal channels using two cross-sectional process models, AquaTellUS and FV-SED, to calculate cross-channel sediment accumulation from river flooding and tidal flooding, respectively. Model outputs are validated by field data collected in the fluvial-dominated and tidally-controlled lower delta plains. Direct sedimentation measurements from the river-dominated lower delta show spatially variable patterns of monsoonal overbank deposition, with localized rates as high as 5 cm/yr. In the tidally controlled western lower delta plain, regional mean accumulation rates are around 1 cm/yr, emphasizing the role of the large (3-4 m) tidal range in sediment dispersal. Seasonal sedimentation patterns revealed by these direct field measurements are comparable to rapid near-channel sedimentation indicated in the modeling results. Using this coupled modeling approach, the unknowns in the flood plain and deltaplain storage terms of the G-B sediment budget are simplified.

#### Modeling the circulation of the NW European shelf seas - present and deep past

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The present day North Sea is here explored through the basic modelling capacities of the Regional Ocean Modeling System (ROMS) coupled with the biogeochemical sub module of Azhar et al., 2014. This new module is capable of investigating low oxygen–anoxic bottom water conditions such as under upwelling or eutrophic systems. The prospect of the study is to provide a ground truth case for the model toward reproducing known circulation, productivity, oxygenation and bottom sediment distribution patterns in the basin, and if successful, to study the effect of predicted sea level change under a changing future climate. These investigations will be used as a back drop for modelling the Cretaceous of Northwest Europe, in order to investigate the effect of climate and bathymetry on productivity, bottom water conditions and carbonate ooze deposition in the region.

#### Hydrological model application and prediction uncertainty analysis

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The main objective of this study was to assess the performance and applicability of the soil water assessment tool (SWAT) model for prediction of streamflow in the Lake Tana Basin, so that the influence of topography, land use, soil and climatic condition on the hydrology of Lake Tana Basin can be well examined. Sequential uncertainty fitting (SUFI-2), parameter solution (ParaSol) and generalized likelihood uncertainty estimation (GLUE) calibration and uncertainty analysis methods were compared and used for the set-up of the SWAT model.

#### Testing bedrock incision models in a mixed bedrock-alluvial system: High Cascades, Oregon

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There is abundant field evidence that sediment supply controls the incision of bedrock channels by both protecting the bed from incision and providing tools to incise the bed. Mixed bedrock-alluvial systems are uniquely suited to test these models, as the transition from bedrock to alluvial morphology can constrain parameters like sediment supply that are otherwise difficult to measure. Here, we use Lidar data and field observations from a fluvial channel cut into a Holocene lava flow in the High Cascades, Oregon to explore the ability of the full physics of models of abrasion by saltating bedload to predict observed incision. The blocky andesite of Collier lava flow erupted from Collier Cone ~1500 years ago, paving over the existing landscape and erasing fine-scale landscape dissection. Since the eruption, a 6 km stream channel has been incised into the lava flow, though the channel is currently dry for most of the year. The channel is comprised of two alluvial reaches and two bedrock gorges. The division between these reaches follows the background slope of the lava flow, with alluvial areas corresponding to low slopes and gorges corresponding to high background slopes. The alluvial reaches are characterized by deposits up to 2 m-thick, and by gravel-bedded self-formed channels; gorges are incised up to 8 m into the flow. Using a simple finite difference scheme with airborne-Lidar-derived preincision topography as an initial condition, we predict incision in the two gorges with the saltation-abrasion model. We examine model outcomes as a function of water discharge, grain size, and sediment supply, fully populating the parameter space with several model runs. Water discharge and grain size are set as free parameters and we use a 1D energy equation to calculate channel shear stress. To constrain sediment supply, we assume that there is no incision in the alluvial reaches, such that sediment supply is greater than or equal to alluvial transport capacity. Our initial results using this approach suggest that for most parameter values, gorge incision is dominated by the tools effect, whereby greater channel shear stress and greater sediment supply result in higher channel incision.

#### The FESD Delta Dynamics Modeling Collaboratory: A Progress Report

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The Delta Dynamics Collaboratory (DDC) is a four-year effort to develop an inter-disciplinary and multi-scale understanding of the interplay among and within the various sub-systems of deltas. It is funded through the National Science Foundation's "Frontiers in Earth System Dynamics" (FESD) Program. The overall objective of the DDC is to develop tested, high-resolution, quantitative models incorporating morphodynamics, ecology, and stratigraphy to predict river delta dynamics over engineering to geologic time-scales. In this way we hope to specifically address questions of delta system dynamics, resilience, and sustainability. There are two laboratories in the DDC: a field laboratory for

discovering process-interactions and testing model predictions (Wax Lake Delta, LA), and a virtual modeling laboratory. Here we report on the progress made to date in advancing models of delta processes and morphodynamic interactions.

The models consist of three types: 1) reduced complexity delta models (RCDM); 2) a 2- and 3D eco-geo-morphodynamic sediment transport delta model; and 3) vegetation and fish population ecological models. The RCDM are focused on large-scale interactions, and as such offer the opportunity to explore aspects of system dynamics that may be harder to pick out of the details of a high-resolution model. "DeltaRCM" is a "2.5-D" cellular delta formation model that computes a depth-averaged flow field and bed topography as the delta evolves in time. The model adopts a Lagrangian view of transport: water and sediment fluxes are treated as a large number of "parcels" that are routed scholastically through a lattice grid. The probability field for routing the parcels is updated through time and is determined by a set of rules abstracting the governing physics of fluid flow and sediment transport. Sediment parcels are treated as "leaking buckets" that lose sediment to the bed by deposition and gains sediment from the bed by erosion. In the current version of the model sediment parcels represent coarse and fine materials respectively ("sand" and "mud"), which have different rules for routing and conditions for deposition and entrainment. DeltaRCM is able to produce delta morphology at the level of selforganized channel behaviors such as bifurcations and avulsions. The model can also record stratigraphy in terms of grain-size or deposition age. Validation work on the flow routing component of the model ("FlowRCM") shows that the model gives reasonable channel-to-channel and channel-to-floodplain flow partitioning but falls short in predicting fine scale hydrodynamic details at fine scales (e.g., sub-channel scale). A second RCDM (Kim et al. 2009) is being modified to include self-formed channels and separate channel and floodplain elevations, treat alluvial-bedrock and bedrock-alluvial transitions in low-slope sand-bed rivers, and exploit new channel geometry closure rules for selfformed alluvial sand-bed channels developed during the course of this study.

Along the lines of reduced complexity models, we have also developed a network-based modeling framework for understanding delta vulnerability to change. The deltaic system is mapped into a directed graph composed of a set of nodes (or vertices) and links (or edges) and represented by its connectivity or adjacency matrix. For flux routing a weighted adjacency matrix is used to reflect how fluxes are split downstream and to enforce mass balance. Using the proper tree representation, we show that operations on the adjacency matrix quantify several properties of interest, such as immediate or distant connectivity, distinct sub-networks, and downstream regions of influence from any point on the network. We use these representations to construct "vulnerability maps", e.g., maps of delta locations where an imposed change in water and/or sediment fluxes would most drastically affect sediment and water delivery to the coastal zone outlets or to a specific region of the delta. Dam construction can be emulated by reducing water and sediment downstream by a given fraction, the location and operation of irrigation dykes can be varied, and different alternative management options can be evaluated in a simple yet spatially extensive framework.

The current open-source state of the art in 3D delta morphodynamic modeling is Delft3DFLOW Version 6.00.00.2367 developed by Deltares, an independent, Dutch-based research institute for matters relating to water, soil and the subsurface (http://www.deltares.nl/en). We are using Delft3D 6.0 to test various hypotheses concerning the emergent behaviors of deltas subject to various sediment fluxes, basin depths, and base level variations, and to investigate the specific morphodynamics and sediment retention of Wax Lake Delta. Predictions of sand and mud transport through the various distributaries compare well with data collected by the FESD Wax Lake Team and indicate that total sediment load is rarely split equally at bifurcations, in accordance with earlier predictions. These and other studies have shown that improvements to Delft3D are needed to solve the following problems: 1) morphodynamic simulations of deltas are in part, an artifact of the underlying orthogonal grid structure; 2) the ecogeomorphic interactions are primitive; 3) the algorithm for eroding channel banks is ad hoc; and 4) simulations are restricted by computational inefficiencies. We are attempting to address these problems in collaboration with Deltares scientists. A mass-conservative, staggered, threedimensional immersed boundary, shallow water Delft3D+ model is under development for flow on complex geometries. It allows channels to evolve independent of the underlying grid, and allows cohesive channel banks to erode laterally according to user-specified bank-erosion rules. The method consists of hybrid cut- ghost-cells: ghost cells are used for the momentum equations in order to prescribe the correct boundary condition at the immersed boundary, while cut-cells are used in the continuity equation to conserve mass. Results show that the resulting scheme is robust, does not suffer any time step limitation for small cut cells and conserves fluid mass up to machine precision. Comparisons with analytical solutions and reference numerical solutions on curvilinear grids confirm the quality of the method.

To improve ecogeomorphic interactions, we have created a sub-grid vegetation-flow interaction module for Delft3D and Delft3D+ based upon the Baptist et al. (2005) equations. Baptist's formulation is based on the theory that vegetation can be modeled as rigid cylinders, which influences the momentum calculation and turbulence structure. Vegetation is characterized by plant height, density, stem diameter, and drag coefficient in the model. The vertical flow velocity profile

is divided into a constant zone of flow velocity inside the vegetated part and a logarithmic velocity profile above for submerged vegetation. Results show that in deltaic freshwater marshes, adding vegetation increases the fraction of sediment deposited inside the marsh but the vegetative roughness also forces more water into the channels, leading to more erosion in the channels and also more water by-passing the marsh surface. Thus under certain conditions, adding vegetation to freshwater marshes can reduce net deposition rates. In addition to the above-ground effects of plants, the role of roots in binding sediment is being modeled in a separate vegetation-root routine through increasing critical shear stress for erosion. When combined flow-wave shear stress is larger than a rooted-soil critical value, aggregate or block erosion occurs. The model is tested against cumulative sediment erosion and deposition on Wax Lake Delta during Hurricane Rita in 2005. The simulation shows that roots significantly change the sedimentation-erosion pattern at the marsh area by protecting the vegetated marshes from erosion.

A fish dynamics model explores the co-evolution of fish populations, vegetation, and delta morphology. The model simulates the individuals of five fish species on a spatial grid of bathymetry, water levels, vegetated habitat, and basal prey. An existing version of this model uses historical water levels, together with fixed bathymetric maps, to determine water depths on each cell and its vegetation type. Model simulations follow each individual of each species through the processes of growth, reproduction, mortality, and movement. Individuals compete for space and invertebrate prey, and individuals of predatory species consume other model individuals. The sum over individuals for a species yields abundances, and the combination of abundance and growth yields productivity. We use the model to identify strong relationships between morphodynamic features (such as mouth bar hypsometry) and predicted total and species-specific fish productivity. As these models reach maturity in the next two years they will be incorporated into the CSDMS architecture and framework. All models will be open source and made freely available via the CSDMS Repository. If you have a specific immediate request please email <u>sling@psu.edu</u>.

#### A new soil-landscape model: focus on its subsurface architecture

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Landscapes are shaped by the combination of (vertical) soil development dynamics and (lateral) geomorphic processes. However, almost all landscape evolution-modeling studies have seen soil as a homogenous quantity: the regolith. This positions geomorphic processes as first-order determinants of landscape forms, and leaves us with questions regarding the relative importance of soil development - despite ample anecdotal evidence of soil-affected geomorphology such as in landscapes with laterite formation or clay translocation. Luckily, some soil-landscape feedbacks are increasingly being included in models of landscape evolution. Here, we present a new 'soilscape' model that combines some parts of the landscale evolution model LAPSUS with most parts of the soil development model of MILESD. Example outputs are presented, but our focus is on the subsoil architecture in the new model, where we compare various alternatives to arrive at our choice: a finite number of layers of variable thickness, variable composition and variable bulk density.

#### How does topography control shallow geological processes?

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Over the past 30 years conceptual and numerical models of crustal evolution have evolved from simple 2D crosssections to complex 3D models that achieve a qualitative, process-based understanding of key aspects of solid earth dynamics. However, recent progress toward improved application of these models to higher spatial and temporal frequencies has revealed considerable inconsistencies in their predictive powers, especially at the near surface. Here we focus on how topography at the scale of ridges and valleys feedback into the 3D stress and strain fields and related parameters. A new formulation, the Failure Earth Response Model (FERM), which unifies the description of tectonic and geomorphic forcings within a single framework, allows us to gather stresses generated by far field tectonics processes, topography and surface processes into a single stress state for every point. We can explicitly consider the contribution that pore pressure fluctuations, seismic accelerations, fault damage and large storm events make toward the rock mass failing using examples from the Southern Alps of New Zealand.
#### Estuarine morphodynamics : better be certain about uncertainty

Mick van der Wegen, UNESCO-IHE & Deltares

Process-based models are able to predict velocity fields, sediment transport and associated morphodynamic developments over time. These models can generate realistic morphological patterns and stable morphodynamic developments over time scales of millennia under schematized model settings. However, more realistic case studies raise questions on model skill and confidence levels. Process-based models require detailed information on initial conditions (e.g. sediment characteristics, initial distribution of sediment fractions over the model domain), process descriptions (e.g. roughness and sediment transport formulations) and forcing conditions (e.g. time varying hydrodynamic and sediment forcing). The value of the model output depends to a high degree on the uncertainty associated with these model input parameters. Our study explores a methodology to quantify model output uncertainty levels and to determine which parameters are responsible for largest output uncertainty. Furthermore we explore how model skill and uncertainty develop over time. We describe the San Pablo Bay (USA) case study and the Western Scheldt (Netherlands) case study in a 100 year hindcast and a more than 100 year forecast. Remarkably, model skill and uncertainty levels depend on model input parameter variations only to a limited extent. Model skill is low first decades, but increases afterwards to become excellent after 70 years. The possible explanation is that the interaction of the major tidal forcing and the estuarine plan form governs morphodynamic development in confined environments to a high degree.

#### Exploring climate mitigation and low-carbon transitions: new challenges for model integration

Alexey Voinov, University of Twente

There are various visions of our future, but most policy-makers and scientists agree that life will be substantially different in the post-fossil era. The cheap and abundant supply of fossil energy has led to unprecedented population growth and to staggering levels of consumption of natural resources, undermining the carrying capacity of nature. Eroding ecosystems, the end of cheap oil and climate change call for new policies to support societal transformations toward low-carbon alternative futures. This understanding has already been expressed in recent EU legislation, which requires that domestic GHG emissions be cut by 80% between 1990 and 2050. Energy is a major driver of change and an important 'currency' that runs economic and social systems and influences environmental systems. Being so used to the abundant and uninterrupted supply of fossil energy, we tend to forget the important role that it plays in our everyday lives. Non-marginal, abrupt changes, such as during the Oil Crisis of the 1970s or the sudden sharp rise in oil prices in 2008 remind us how vulnerable societies are with respect to energy. Future transitions and climate induced changes are also unlikely to be smooth and require new modeling paradigms and methods that can handle step-change dynamics and work across a wide range of spatio-temporal scales, integrating the knowledge of many stakeholder communities.

Here we are operating in a generalized 'socio-environmental model space', which includes empirical models, conceptual stakeholder models, complex computer simulations, and data sets, and which can be characterized in several dimensions, such as model complexity, spatial and temporal resolution, disciplinary coverage, bias and focus, sensitivity and uncertainty, usability and relevance. In this space we need a 'model calculus' – a set of relationships and operations that can apply to individual models and groups of models. Model integration across disciplinary boundaries faces two big challenges. First we need to learn to deal with a variety of modeling paradigms and techniques, allowing different types of models to exchange information in a meaningful way (agent based models talk to systems dynamics, to computed global equilibrium models, to empirical models, etc.). Secondly, we need to provide integration techniques and tools that bring qualitative, conceptual, mental models of stakeholders together with the quantitative simulation models.

Greater transparency and accessibility can be achieved through enhancing documentation and communication of model functioning and strengths and limitations of various models and approaches. This extensive model documentation following improved and enhanced meta model standards is an important first step that makes sure that models (both qualitative and conceptual) 'talk the same language' and can exchange information and knowledge at various stages of research. This also helps us create the ontology, which can be further used for computer aided semantic mediation of models. This semantic mediation should include such functionality as consistency checks (checking for units, concepts, spatio-temporal resolution, etc.). This should also help to explore the different models along the complexity continuum to understand how information from more aggregated qualitative models can be transmitted to more elaborated and detailed quantitative simulations, and vice versa. This bears the promise of insight on the complex behavior of non-linear systems where regime shifts and non-equilibrium dynamics is usually better understood with simple models, while the more complicated models are easier to parametrize with data and can take into account more detailed information about particular systems and situations.

#### Water and sediment discharge into the sea from Yangtze River: an improving measurement

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One third of the world population lives in the coastal zone whose natural environment and ecosystems are directly impacted by the freshwater and sediment discharged by the rivers. Yet, the conventional method to estimate the river discharges is based on the record of the gauging station located closest to the river mouth, which could be hundreds of kilometers away; such a method is insufficient to produce accurate values. Here we present in-situ yearlong observations of the water and sediment discharges through a cross-section near the mouth of the Changjiang (Yangtze River). This data was first compared to the data obtained from the nearest river gauging station at Datong, and then used to derive two methods to accurately estimate the water and sediment discharges of the entire drainage basin.

# Integrating glaciers and isostatic deformation into Landlab, a computational framework for Earth-surface systems

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Landlab is a new modeling framework to integrate components of the Earth-surface system and understand their interactions. Here we add two new components: (1) a mechanical ice flow model and (2) a model of Earth's flexural isostatic response to surface loads. The two are fully coupled, as large ice masses produce significant deflections of the surface. The mechanical ice flow model calculates 2D (depth-averaged) horizontal ice fluxes in response to an evolving surface mass balance parameterization and prescribed isothermal ice temperature. Solving depth-integrated ice velocity under prescribed ice temperature provides sufficient computational efficiency, relative to a fully 3D thermo-mechanical ice flow model, to explore glacier form and flow on geologic timescales. The flexure model ingests load distributions and a prescribed map of lithospheric elastic thickness to produce surface deflections. These connect with GRASS GIS to act as a database and platform for data–model integration and bypass the need to prepare input files. We explore the fully-transient interplay between ice overburden and lithospheric flexure using as a case study the evolution of the Yellowstone ice cap over the last glacial cycle, which covered an area of ~40,000 km2 at the Last Glacial Maximum (~26.5–19.5 ka).

#### Hydrodynamics and morphological changes of the Wax Lake Delta (WLD) during hurricane Rita, 2005

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For this study Delft3D HD module, coupled with SWAN and a morphology module is applied to explore the impact of hurricane Rita (2005) on the hydrodynamics and morphological changes of WLD, A vegetation routine is also incorporated to study the influence of plants during this hurricane event. Under normal conditions tides cause water level to change by  $\sim 1$  m (-0.5  $\sim 0.5$  m). During hurricane Rita, the storm surge causes water level to rise to as high as 3 m. Water level at the deltaic area first decreases by more than 2 m before the hurricane storm surge approaches while water accumulates towards the center of the hurricane. Current velocity at the deltaic area increases from 0.6 m/s (during tides) to 1.5 m/s (during hurricane Rita), and the storm surge causes water to flow upstream in the river channels, lasting for 12 hours. Simulation results without including a vegetation routine reveal that after hurricane Rita made landfall, the delta morphology changed such that sediments eroded mostly on the deltaic islands and were

deposited in the distributary channels. This demonstrates an opposite pattern to former observations made during river floods, indicating that hurricanes decrease the progradation of WLD. A model simulation incorporating aboveground vegetation shows that plants reduce storm surge progradation, and diminish the impact of hurricane Rita on the deltaic area such that the vegetated islands are less eroded. Less sediment is deposited in the distributary channels as well. The impact of plant roots has been explored through stabilizing bed materials, both for cohesive and non-cohesive sediments. Results demonstrate that roots can significantly decrease erosion in vegetated areas and illustrates that vegetation could be a great protector to wetlands, especially during extreme events.

#### Predictions of bedload transport in vegetated channels: uncertainties and steps forward

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Vegetation in river channels and on floodplains alters mean flow conditions, turbulence, sediment transport rates and local sedimentation patterns. Although many advances have been made to predict the impact of vegetation on flow conditions, relatively few studies have investigated how vegetation influences bedload fluxes. We first investigate how known vegetation impacts on flow turbulence can be used to better predict bedload transport and sedimentation within vegetation patches. To elucidate these mechanics we measured 2D velocity fields using PIV and bedload fluxes using high-speed video in simplified flume experiments. We used these laboratory measurements to test and develop bedload transport equations for vegetated conditions. Bedload transport equations did not accurately predict sediment fluxes unless they accounted for the spatial variability in the near-bed Reynolds stress. We then use this patch scale understanding to better predict how vegetation impacts channel morphology. Specifically, we investigate how vegetation influences point bar growth and shape through coupled laboratory experiments and 2D numerical modeling. We measured bedload fluxes, flow conditions and sedimentation rates on a point bar planted with natural vegetation at the Saint Anthony Falls Outdoor Stream Lab. We then calculated the detailed 2D flow field over the point bar throughout imposed flow hydrographs. Our results demonstrate that vegetation caused significant changes in the bar dimensions and depending on the flow level, led to the development of a side channel between the bar and the inner bank of the meander. Such a side channel could precipitate a change in channel morphology to a multi-thread channel. Accurate predictions of sedimentation caused by vegetation patches not only require an estimate of the spatial variation in shear stress (or velocity) within a patch but also how the vegetation alters the adjacent flow field and bedload sediment supply to the patch.

# Parameter and model uncertainty analysis of a physics-based hydrologic model: a comparative study of GLUE and Gaussian process emulator

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Quantification of uncertainty of environmental models plays an important role in the decision making process. The most popular method GLUE (Generalized Likelihood Uncertainty Estimation) has been argued for the computationally inefficiency due to the emerging of complex models. Recently, the Bayesian approach using Gaussian process (GP) emulator has been attracted much attention in the uncertainty analysis of computationally expensive models. It would be useful to compare the difference of this two methods in the uncertainty analysis of a physics-based hydrologic model. We evaluate the difference of GLUE and GP emulator in the assessment of parameter uncertainty of a physics-based integrated hydrologic model (Penn State Integrated Model: PIHM). PIHM integrates the hydrological processes including interception, throughfall, infiltration, recharge, evapotranspiration, overland flow, groundwater flow, and channel routing, in a fully coupled scheme. The tradition parameter estimation focuses only on the model performance at streamflow, which may cause significant uncertainty of parameter in other intermediate predicted variables (groundwater table, soil moisture, etc.). We demonstrate the uncertainty at each process to investigate the uncertainty transfer in the integrated framework of PIHM. This study considers the comparison between GLUE and GP emulator uncertainty analysis at a catchment at central PA: Shale Hills, where hydrologic processes are monitored, including intermediate variables of rainfall-runoff processes. The GLUE method attempts to evaluate the total uncertainty from model structure, parameter, and input data through a large sample of model simulation. Whereas, the GP emulator starts with designed samples of model runs, and allows inferring the values of the model output at untried points. The

uncertainty disentanglement between model structure, parameter, and hydrologic processes suggests that ignoring intermediate variable uncertainty will lead to unrealistic model simulations.

#### Fully-Coupled Hydrologic-Morphologic Processes for Modeling Landscape Evolution

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Investigating the impacts of properties, distribution and evolution of regolith on river channel, fluid pathways, flow rate and sediment transport is essential to resource management and restoration efforts. Besides field experiment studies, numerical simulation is also an efficient way to explore the relationship between the hydrological and morphological processes. Recent studies focus more on the interaction of physical processes that govern the surface hydrodynamics and morphodynamics. However, the fluid flow on the subsurface layer plays an important role on landscape evolution as well. This study takes into account of the water exchange between surface and subsurface and water flow within subsurface and fully couples them into a 3D hydrologic-morphodynamic model (LE-PIHM) for regolith formation and landscape evolution by using finite volume strategy. Two scenarios, coupling subsurface flow and no subsurface flow, are applied in a synthetic experiment. A comparison of the simulation results in the two scenarios at steady state indicates that subsurface flow has significant influences on the distribution of regolith, steepness of hillslope, network density, drainage area and water balance.



Photo: CSDMS Annual Meeting 2014 Poster Session

# Appendix 3: 2013 CSDMS Annual Meeting Clinics

#### **SNAC: A 3D parallel explicit finite element code for long-term lithospheric deformation modeling** Eunseo Choi, Center for Earthquake Research and Information, University of Memphis

SNAC (StGermaiN Analysis of Continua) is a 3D parallel explicit finite element code for modeling long-term deformations of lithosphere. It is an open source being distributed through Computational Infrastructure for Geodynamics (http://geodynamics.org/cig/software/snac/) as well as through CSDMS web site (http://csdms.colorado.edu/wiki/Model:SNAC). This clinic will provide an overview of SNAC and lead participants through a typical work procedure for producing a 3D lithospheric deformation model on a high performance cluster. Specifically, participants will take the following steps: 0) acquiring an account on the CSDMS HPC (to be done before the clinic); 1) checking out the source code through a version control system; 2) building SNAC on the cluster; 3) getting familiar with SNAC by running a cookbook example in parallel and visualizing outputs; 4) modifying the source codes to customize a model.

#### Sediment Transport in an Idealized Domain Using ROMS

Courtney Harris, VIMS

Participants in this clinic will learn how to compile and run a Regional Ocean Modeling (ROMS) test case for an idealized continental shelf. The hydrodynamic model that we will use includes wave forcing and suspended sediment transport. ROMS is an open source, three-dimensional primitive equation hydrodynamic ocean model that uses a structured curvilinear horizontal grid and a stretched terrain following vertical grid. For more information see https://www.myroms.org. It currently has more than 4,000 registered users, includes modules for sediment transport and biogeochemistry, and has several options for turbulence closures and numerical schemes. Model input is specified using a combination of ASCII text files and NetCDF (Network Common Data Form) files. Output is written to NetCDF files. In part because ROMS was designed to provide flexibility for the choice of model parameterizations and processes, and to run in parallel, implementing the code can seem daunting, but in this clinic we will present an idealized ROMS model that can be run on the CSDMS cluster. As a group, we will compile and run an idealized ROMS model on the CSDMS computer, Beach. The group will choose a modification to the standard model. While the modified model runs, we will explore methods for visualizing model output. Participants who have an account on Beach can try to run the model themselves. Clinic participants who have Matlab set up to visualize NetCDF files will be able to browse model output files during the clinic. Following the clinic, participants should have access to tools for looking at ROMS output, an example ROMS model run, and experience with ROMS input and output files.

#### Carbonate Models Clinic - carbo\* suite

Chris Jenkins, INSTAAR

The carbo\* set of modules uses Lotka-Volterra population ecology, hydrodynamics, mesoscale simulators, an organism knowledge base (OKB), and habitat suitability indexes to model benthic carbonate production. The modeling covers coral reef, Halimeda and maerl, oyster, deep-water coral and bryozoan facies but can be extended to other types using the OKB. Recently the creation of rubble bioclasts has been addressed by modeling bioerosion, skeleton breakage, water column turbulence statistics, and clast ballistic trajectories in extreme weather. Model runs are initiated for modern situations by automatically gathering data from global database and remote sensed resources such as MODIS AQUA, World Ocean Atlas, WaveWatch, GEBCO. Idealized scenarios – from paleogeography - can also be constructed and submitted for modeling. Time spans of up to 10,000 years have been run, using a burst technique with annual time-stepping. Seasonal stepping for shorter time span is also possible. The model outputs include profiles of organism biofacies, accumulation geometries, (1m3) 'block of rock' fabric & porosity models for generated materials, and 3D and animated mappings of the sediment facies.

The clinic will go through a typical setup and run, with some variations within the group. One of the modeled areas will be Molokai, Hawaii. Participants on the day will receive a copy of the software. Images of recent outputs are shown at [http://instaar.colorado.edu/~jenkinsc/carboClinic2014/carboClinicImages2014.htm http://instaar.colorado.edu/~jenkinsc/carboClinic2014/carboClinicImages2014.htm]. Future developments will be discussed, particularly integration with terrigenous sediment and suspendate models, and nutrient loadings.

# The SAFL Virtual StreamLab (VSL3D): High Resolution Simulation of Turbulent Flow, Sediment Transport, and Morphodynamics in Waterways

Ali Khosronejad, University of Minnesota

The St. Anthony Falls Laboratory Virtual StreamLab (VSL3D) is a powerful multi-resolution and multiphysics Computational Fluid Dynamics (CFD) model for simulating 3D, unsteady, turbulent flows and sediment transport processes in real-life streams and rivers with arbitrarily complex structures, such as manmade hydraulic structures, woody debris, and even hydrokinetic turbine arrays. The code can handle arbitrarily complex geometry of waterways and embedded structures using novel immersed boundary strategies. Turbulence can be handled either via Reynolds-averaged Navier-Stokes (RANS) turbulence models or via large-eddy simulation (LES) coupled with wall models. Free-surface effects are simulated using a level-set, two-phase flow approach, which can capture complex free-surface phenomena, including hydraulic jumps, over arbitrarily complex bathymetry. A fully-coupled hydro-morphodynamic module has also been developed for simulating bedload and suspended load sediment transport in meandering rivers. A novel dual time-stepping quasi-synchronized approach has been developed to decouple the flow and sediment transport time scales, enabling efficient simulations of morphodynamic phenomena with long time scales, such as dune migration in rivers. The code is parallelized using MPI. This clinic will present a comprehensive overview of the VSL3D, report extensive grid sensitivity and validation studies with experimental data, and present a series of applications, including: 1) LES and unsteady RANS of turbulent flow and scalar transport in natural meandering streams; 2) LES of sand wave growth and evolution in a laboratory scale flume; 2) unsteady RANS of dune formation and migration in large scale meandering rivers with in stream rock structures (rock vanes, j-hooks, w-weirs, etc.); 3) LES of free-surface flows in natural and enginnered open channels; and 4) LES of gravity currents.

#### Interactive Data Analysis with Python

Monte Lunacek, University of Colorado

Recent additions to Python have made it an increasingly popular language for data analysis. In particular, the pandas library provides an R-like data-fame in Python, which is data structure that resembles a spreadsheet. This provides an efficient way to load, slice, reshape, query, summarize, and visualize your data. Combining this with numpy, maplotlib, and scikit-learn creates a powerful set of tools for data analysis. In this hands-on tutorial, we will cover the basics of numpy, matplotlib, pandas, and introduce scikit-learn.

#### Introduction to the Basic Model Interface and CSDMS Standard Names

Scott Peckham, University of Colorado

In order to simplify conversion of an existing model to a reusable, plug-and-play model component, CSDMS has developed a simple interface called the Basic Model Interface or BMI that model developers are asked to implement. In this context, an interface is a named set of functions with prescribed function names, argument types and return types. By design, the BMI functions are straightforward to implement in any of the languages supported by CSDMS, which include C, C++, Fortran (all years), Java and Python. Also by design, the BMI functions are noninvasive. A BMI-compliant model does not make any calls to CSDMS components or tools and is not modified to use CSDMS data structures. BMI therefore introduces no dependencies into a model

and the model can still be used in a "stand-alone" manner. Any model that provides the BMI functions can be easily converted to a CSDMS plug-and-play component that has a CSDMS Component Model Interface or CMI. Once a BMI-enabled model has been wrapped by CSDMS staff to become a CSDMS component, it automatically gains many new capabilities. This includes the ability to be coupled to other models even if their (1) programming language, (2) variable names, (3) variable units, (4) time-stepping scheme or (5) computational grid is different. It also gains (1) the ability to write output variables to standardized NetCDF files, (2) a "tabbed-dialog" graphical user interface (GUI), (3) a standardized HTML help page and (4) the ability to run within the CSDMS Modeling Tool (CMT). This clinic will explain the key concepts of BMI, with step-by-step examples. It will also include an overview of the new CSDMS Standard Names, which provide a standard way to map input and output variable names between component models as part of BMI implementation. Participants are encouraged to read the associated CSDMS wiki pages in advance and bring model code with specific questions.

# WMT: The CSDMS Web Modeling Tool

Mark Piper, Irina Overeem, & Eric Hutton, CSDMS, University of Colorado

The CSDMS Web Modeling Tool (WMT) is the web-based successor to the desktop Component Modeling Tool (CMT). WMT presents a drag-and-drop interface that allows users to build and run coupled surface dynamics models from a web browser on a desktop, laptop or tablet computer.

With WMT, a user can:

- Design a coupled model from a list of available components
- Edit the parameters of the model components
- Save the coupled model to a server, where it can be accessed from any computer
- Set run parameters, including the computer/cluster on which to run the model
- Share saved modeling projects with others in the community
- Submit jobs to the high-performance computing system

Although WMT is web-based, the building and configuration of a model can be done offline. The user can then reconnect to save a model and submit it for a run. In this clinic we present an overview of WMT, including an explanation of the user interface, a listing of the currently available models and a discussion of how models can be run in operational mode or in reduced-input mode for teaching. We cap the clinic with a live demonstration of setting up, saving and running a coupled model on the CSDMS supercomputer system.

#### Dakota: A Toolkit for Sensitivity Analysis, Uncertainty Quantification, and Calibration

Laura Swiler & J. Adam Stephens, Sandia National Laboratories

Dakota is an open-source toolkit with several types of algorithms, including sensitivity analysis (SA), uncertainty quantification (UQ), optimization, and parameter calibration. Dakota provides a flexible, extensible interface between computational simulation codes and iterative analysis methods such as UQ and SA methods. Dakota has been designed to run on high-performance computing platforms and handles a variety of parallelism. In this clinic, we will provide an overview of Dakota algorithms, specifically focusing on uncertainty quantification (including various types of sampling, reliability analysis, stochastic expansion, and epistemic methods), sensitivity analysis (including variance-based decomposition methods and design of experiments), and parameter calibration (including nonlinear least squares and Bayesian methods). The tutorial will provide an overview of the methods and discuss how to use them. In addition, we will briefly cover how to interface your simulation code to Dakota.

# Creative computing with Landlab: A flexible Python package for rapidly building and exploring 2D surface-dynamics models

Greg Tucker & Daniel Hobley, CIRES

Computer models help us explore the consequences of scientific hypotheses at a level of precision and quantification that is impossible for our unaided minds. The process of writing and debugging the necessary code is often time-consuming, however, and this cost can inhibit progress. The code-development barrier can be especially problematic when a field is rapidly unearthing new data and new ideas, as is presently the case in surface dynamics. To help meet the need for rapid, flexible model development, we have written a prototype software framework for two-dimensional numerical modeling of planetary surface processes. The Landlab software can be used to develop new models from scratch, to create models from existing components, or a combination of the two. Landlab provides a gridding module that allows you to create and configure a model grid in just a few lines of code. Grids can be regular or unstructured, and can readily be used to implement staggered-grid numerical solutions to equations for various types of geophysical flow. The gridding module provides built-in functions for common numerical operations, such as calculating gradients and integrating fluxes around the perimeter of cells. Landlab is written in Python, a high-level language that enables rapid code development and takes advantage of a wealth of libraries for scientific computing and graphical output. Landlab also provides a framework for assembling new models from combinations of pre-built components. In this clinic we introduce Landlab and its capabilities. We emphasize in particular its flexibility, and the speed with which new models can be developed under its framework. In particular, we will introduce the many tools available within Landlab that make development of new functionality and new descriptions of physical processes both easy and fast. Participants will finish the clinic with all the knowledge necessary to build, run and visualize 2D models of various types of earth surface systems using Landlab.

#### Agent-Based Modeling Research: Topics, Tools, and Methods

Joshua Watts, Arizona State University

Agent-Based Modeling (ABM) or Individual-Based Modeling is a research method rapidly increasing in popularity -- particularly among social scientists and ecologists interested in using simulation techniques to better understand the emergence of interesting system-wide patterns from simple behaviors and interactions at the individual scale. ABM researchers frequently partner with other scientists on a wide variety of topics related to coupled natural and human systems. Human societies impact (and are impacted by) various earth systems across a wide range of spatial and temporal scales, and ABM is a very useful tool for better understanding the effect of individual and social decision-making on various surface processes. The clinic will focus on introducing the basic toolkit needed to understand and pursue ABM research, and consider how ABM work differs from other computational modeling approaches. The clinic: - Will explore examples of the kinds of research questions and topics suited to ABM methods. - Will (attempt to) define some key concepts relevant to ABM research, such as emergence, social networks, social dilemmas, and complex adaptive systems. - Will provide an introduction to ABM platforms, particularly focused on NetLogo. - Discuss approaches to verification, validation, and scale dependency in the ABM world. - Introduce the Pattern-Oriented Modeling approach to ABM. - Discuss issues with reporting ABM research (ODD specification, model publishing). - Brainstorm tips and tricks for working with social scientists on ABM research

# Appendix 4: 2014 CSDMS Annual Meeting Awards

The 2014 CSDMS Lifetime Achievement Award in Earth Surface Dynamics Modeling was presented to Professor Patricia Wiberg (UVA) in Boulder Colorado, as part of the 2014 CSDMS Annual Meeting. Presenters included Professor Courtney Harris, Professor Jim Smith, and Professor James Syvitski.



Dedication: "Professor Wiberg is both a pioneer and world leader on the subject of marine, coastal and fluvial sediment transport. She has approached this field from every conceivable methodology and theoretical construct, from in situ field and flume measurements, to ecogeomorphodynamics, geotechnical analysis, boundary layer oceanography, and numerical modeling approaches. These efforts have resulted in a well-cited suite of papers that encapsulate our understanding of how fluids under various forcing conditions (windwaves, geostrophic currents, fluid mud, tidal motion, tsunamis waves) can erode the bed and transport this sediment to less energetic environments." - James Syvitski, CSDMS Executive Director

Photo: Professor Wiberg (left) receives a one of a kind art piece from Professor Syvitski (right).

The 2014 CSDMS Best Poster Award went to Jaap Nienhuis for his submission, "Wave angle control on deltaic channel orientation."



Photo: Jaap Nienhuis received a Kindle for Best Poster



# 2013 CSDMS Student Modeler of the Year Award



CSDMS Student Modeler of the Year Award for 2013 was awarded to **Ajay Limaye** (CalTech) for his submission, "A vector-based method for bankmaterial tracking in coupled models of meandering and landscape evolution."

Ajay Limaye, a Phd student with Mike Lamb at the California Institute of Technology, presented a new vector-based method to keep track continuously of eroded and accreted sediment. This new method allows feedback between bank strength and channel migration rates without discretizing the substrate properties and provides distinct advantage to previous efforts.

Photo: Dr. Irina Overeem presented Limaye with the 2013 Student Modeler Award

# Appendix 5: CSDMS Special issue: Uncertainty and Sensitivity in Surface Dynamics Modeling

To be published in Elsevier's Computers & Geosciences. Expected publication date: winter 2015 – early spring 2016. In the special issue we will highlight in its broadest form the following that can affect model simulations:

- Uncertainties associated with model input data and how the data captures natural variability
- Internal model uncertainty resulting from both model simplification which generates uncertainty at all levels, and modeling schemas which have their own unique numerical solution and resolution limitations
- Error propagation between coupled models. Some exchange variables may have their uncertainties dampened in contrast to others where they are amplified.
- Test/verification data used to judge model performance, either field or lab, all come with their own uncertainties. Sensitivity analysis can help determine where effort should be placed.

Nr.	Corresponding author & proposed co-authors	Working title
1	Young Gu Her	Uncertainty of a Grid-based Distributed Hydrology and Sediment Transport Model
2	Z. Cheng, X. Yu, <b>TJ. Hsu</b>	A numerical investigation of fine sediment resuspension wave boundary layer uncertainties in turbulence modulation and hindered settling
3	<b>Brad Murray</b> , Nicole Gasparini, Mick van der Wegen, Evan Goldstein	Certain Uncertainties and Uncertain Uncertainties: It's easier to quantify uncertainty for some models than for others
4	S. Mostafa Siadatmousavi & Felix Jose	Uncertainties in the Third Generation Phase-Averaged Wave Models
5	Matthias vanmaercke, Jean Poesen, Gerard Govers	A methodology to estimate the total uncertainty on average sediment export measurements
6	Attila Lazar, R.J. Nicholls, D. Clarke, P.G. Whitehead, M. Salehin, A. Haque, A.R. Akanda, L. Bricheno, P. Challenor	Error propagation and uncertainty in a coupled model of agricultural production in the delta regions of Bangladesh
7	<b>Jennifer Jefferson</b> , Paul Constantine and Reed Maxwell	Influence of surface and subsurface parameter uncertainty and sensitivity on the latent heat flux using an integrated hydrologic model
8	Decian Valters	Modeling Landscape Sensitivity to Storminess and Climatic Variation
9	Arnaud Temme Tom Van Wallenghem	Combined soil-landscape modelling: effects of changes in climate and human activity on soilscapes.
10	<b>Fedor Baart</b> , Mark Koningsveld, Jaap van Thiel de Vries, Maarten van Ormondt	Confidence in real-time forecasting of morphological storm impact
11	<b>Shawn Harrison</b> , K.R. Gryan, J.C. Mullarney	Uncertainty in modeling a simplistic ebb-jet with opposing waves
12	<b>Giovanna Pisacane</b> , B. Fekete, M.V. Struglia	On the effects of bias correcting the driving temperature and precipitation fields on the hydrological response of European

The following people committed to contribute to the special issue:

		catchments as simulated by a distributed hydrological model.
13	<b>Sofia Pechlivanidou</b> , Patience Cowie, Bjarte Hannisdal and Rob Gawthorpe	Controls on deltaic sedimentation in an active rift setting: an example from Sperchios delta, central Greece
14	Getachew Belete, Alexey Voinov	Exploring temporal and functional synchronization in integrated models
15	Mick van der Wegen	Data assimilation in estuarine morphodynamic modeling
16	E. Mockler, Michael Bruen	Sensitivity analysis of a hydrology/contaminant model to inform parameter regionalisation for unmonitored catchments.
17	Nicole Gasparini, Daniel Hobley, Gregory Tucker, Erkan Istanbulluoglu, Jordan Adams, Sai Nudurupati, and Eric Hutton	Calibrating and validating landscape evolution models: examples using the CHILD and Landlab models
18	Jaeho Shim, Jennifer Duan	Experimental Measurements of Stochastic Bed Load Transport
19	<b>Peter Koons</b> , Phaedra Upton, Samuel Roy, Greg Tucker	Uncertainty in prediction of knickpoint migration arising from divergent theoretical constructs
20	Anna Kelbert, Mary Hill, <b>Scott</b> <b>Peckham</b> and Eric Hutton	Model uncertainty and parameter estimation components in an Earth system modeling framework environment
21	Sean Smith, Andrew Reeve, Brett Gerard, Danielle Martin and Brian Van Dam	Parameter lumping implications to surface runoff simulations designed for watershed sustainability applications in post-glacial terrain of Northeastern U.S.A.
22	Gerben J. de Boer, F. Baart, J. Boerboom	Validation of tidal models using Web Processing Service tidal analysis and prediction
23	<b>Xuan Yu,</b> Anna Lamačová, Christopher Duffy, Pavel Krám, Jakub Hruška	Hydrological model uncertainty due to spatial evapotranspiration estimation methods
24	<b>Greg R. Hancock,</b> T.J. Coulthard, and J.B.C. Lowry	Predicting uncertainty in sediment transport and landscape evolution – an examination of the role of initial landscape conditions

# Appendix 6: Towards Improved Uncertainty Quantification for Earth System Models

S.D. Peckham, CSDMS, U. Colorado, Boulder CO, USA

# 1. Introduction and Purpose

One of the major goals of the second, five-year funding phase of the CSDMS project (Community Surface Dynamics Modeling System) is to provide tools that can be used to better understand and quantify uncertainty in Earth surface process models. In an earlier scoping exercise and literature review by the author, DAKOTA was identified as a promising candidate for helping to fulfill this goal. DAKOTA is attractive for the following main reasons: (1) it uses a liberal, open-source license (LGPL for version 5 and higher), (2) it is mature, long-lived and well-supported (used extensively within DOE and elsewhere), (3) it is component-based, (4) it is extensible and already provides convenient, one-stop access to a large number of third-party libraries for uncertainty quantification, (5) many new features are planned for future releases, (6) it is well-documented and (7) most of its algorithms can automatically make use of multiple processors in a high-performance computing (HPC) environment.

While DAKOTA appears to be a sound choice for some sort of inclusion in CSDMS, there remains the question of how best to integrate it into the system, in view of the current capabilities of the CSDMS modeling framework and its use of standardized interfaces such as the Basic Model Interface (BMI). This represents the *technical challenge* of bringing uncertainty quantification into CSDMS. While the componentization of models in CSDMS and the use of standard interfaces and service components will all help to facilitate this integration, there are still challenges that must be overcome. One of the key challenges is how to create a service component that can retrieve the information from a model that is needed to compute the derivatives of an objective function, since these are needed for model calibration and gradient-based optimization. Forward models (as opposed to inverse models) are usually not written to provide these derivatives, and while *numerical differentiation* is an option, *automatic differentiation* (explained later) provides superior results but may require invasive changes to the source code of models.

Beyond the technical challenges there are also *social challenges* that must be overcome. Virtually all of the models in CSDMS repository so far are *forward models*, and forward modelers tend to be much less familiar with the concepts and algorithms that are used for uncertainty quantification. By contrast, inverse modelers – notably those from the deep-earth process (geodynamics), groundwater and ice sheet modeling communities – tend to be much more familiar and comfortable with these concepts. In view of this, CSDMS will need to budget resources not only for the technical task of integrating DAKOTA into CSDMS, but also for building up the interest and background knowledge that will be needed before its primary user base (surface process model developers and users) begin to use the new capabilities. This represents something of a cultural shift that may be difficult to instigate within this community of modelers.

The three key goals or purposes of this document are therefore to:

- Provide a convenient overview for geoscience modelers of a range of uncertainty topics (especially for forward vs. inverse modelers).
- Provide an overview of the extensive capabilities of the DAKOTA software package and the various ways it can be connected to models.
- Provide guidance with regard to extensions that can be made to CSDMS in order to better support Uncertainty Quantification, particularly with regard to DAKOTA.

#### 2. Background: Key Concepts and Terms

#### 2.1. Optimization Methods

Optimization methods seek to find points in (design) parameter space for which some *objective function* attains either a local or global extrema. The objective function may represent a cost, loss or penalty that is to be minimized, or some reward that is to be maximized. Often an objective function is used to characterize the goodness of a particular design or solution that is being sought. It may also be used as a metric (e.g. the sum

of squared differences function) to measure the "distance" between observed and predicted, or actual and target values. Optimization methods are therefore also required for model calibration, model fitting (e.g. curve and surface fitting), and inverse modeling.

A classic test problem in the field of *mathematical optimization* is to find the global minimum of the *Rosenbrock function*. This function, also know as Rosenbrock's valley or Rosenbrock's banana function, is given by:

$$f(x, y) = (a - x)^2 + b(y - x^2)^2$$

The global minimum of this function occurs at  $(x,y) = (a, a^2)$ , where f(x,y) = 0. Typically one takes a = 1 and b = 100. This problem is illustrative and provides a good test of an optimization algorithm because the global minimum lies along the bottom of a long, narrow valley that has a parabola-shaped cross-section and a very flat bottom. While it is easy for algorithms to find the valley, it is difficult to converge to the location of the global minimum within this valley. The Rosenbrock function, shown in Figure 1, is also used as an example in the DAKOTA package.



Figure 1. The Rosenbrock function, a classic test problem in optimization.

#### Gradient-Based Optimization

Many models of physical processes are based on mathematical functions that have continuous first and second derivatives. In addition, many optimization problems can be formulated in terms of cost (or penalty) functions that have continuous first and second derivatives. For these types of models, it is often possible to find local extrema (stationary points) of the function using standard methods of calculus, i.e. by determining locations where derivatives are equal to zero. A second derivative test can then be used to determine whether a minimum or maximum occurs at that location. Gradient-based local methods include: Conjugate Gradient, Sequential Quadratic Programming (SQP), Newton Methods and Method of Feasible Directions (MFD). (Also Adjoint Equation and Steepest Descent.)

Gradient-based optimization algorithms require computing the *gradient* and/or *Hessian* of an *objective function*. The *gradient* is the vector of first derivatives of the objective function with respect to each of the continuous design variables (those that can be varied to improve the design). The *Hessian* is the square matrix of mixed second derivatives with respect to all of the continuous design variables. It captures the local curvature of the objective function at each point in the parameter space. If the objective function of the design variables/parameters is denoted as:  $f(x_1, x_2, ..., x_n)$ , then the Hessian matrix is given by:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

There are three distinct types of differentiation that can be used to compute the gradient and Hessian of an objective function for use with gradient-based optimization algorithms. In some cases these derivatives can be computed by *symbolic differentiation* using the chain rule, and model code can be written to return the resulting functions evaluated at required points in the parameter space. Derivatives can also be estimated using *numerical differentiation*, in which derivatives are approximated using values in neighboring grid cells (based on some kind of stencil) and the grid cell dimensions (e.g. the method of finite differences). The third type of differentiation. It exploits the fact that every computer program, no matter how complicated, performs calculations by combining elementary arithmetic operations (addition, subtraction, multiplication, division, powers, etc.) with evaluations of elementary functions (exp, log, sin, cos, etc.). By applying the chain rule to this sequence of operations it is possible to automatically compute derivatives of arbitrary order that are accurate to the machine's working precision while using only a small constant factor more operations than the original program.

Note that most Earth system models (*forward models* in particular) compute their output variables without utilizing an objective function and therefore have not been written to be able to return the derivatives of their variables. In order to use gradient-based optimization algorithms with such models, additional software components/utilities of some kind will therefore be required that can compute the required derivatives, hopefully in a way that is noninvasive and does not require major changes to the models themselves. By contrast, *inverse models* usually specify an objective function and are therefore usually able to compute estimates of its derivatives.

#### Derivative-Free Local Optimization

Derivative-free local methods do not require computing derivatives of the objective function and can therefore be used for a larger class of optimization problems where continuous derivatives may not exist (including problems with discrete parameters). These methods use a variety of different algorithms for searching the parameter space for optimal solutions and for refining or focusing the search in the vicinity of good solutions to find better solutions. Examples include: Pattern Search methods (e.g. Asynchronous Parallel Pattern Search, COLINY Pattern Search and Mesh Adaptive Search), Simplex methods (e.g. Parallel Direct Search, COBYLA and Nelder-Meade) and Greedy Search Heuristic (e.g. Solis-Wets method).

# Derivative-Free Global Optimization

Derivative-free global methods do not require computing derivatives of the objective function and can therefore be used for a larger class of optimization problems where continuous derivatives may not exist. Examples include: Evolutionary Algorithms (EA) which are based on concepts from Darwin's Theory of Evolution and concepts from genetics such as natural selection, reproduction, mutation, crossover, inheritance and recombination (e.g. coliny\_ea, soga and moga in DAKOTA) and Division of RECTangles (DIRECT) (e.g. ncsu\_direct and coliny\_direct in DAKOTA.)

#### Population-Based Optimization

Examples include: Genetic Algorithms (e.g. from the larger class of Evolutionary Algorithms), Memetic Algorithms (based on the concept of *memes*, which combine an evolutionary or population-based algorithm

with individual learning or local improvement procedures), Swarm Algorithms (e.g. Ant Colony Optimization, Particle Swarm Optimization, Intelligent Water Drops), Harmony Search, Cuckoo Search and Differential Evolution.

# Other Optimization Methods

Examples include: Simulated Annealing, Random Search, Direct Search, Grid Search and IOSO (Indirect Optimization based on Self-Organization).

# 2.2. Model Calibration

Model calibration involves minimization of an *objective function* that provides a measure (or metric) of the discrepancy between sets of observed and model-predicted values. Model calibration is also used for inverse modeling problems.

**Nonlinear Least Squares.** While any optimization algorithm can be applied to a model calibration problem, nonlinear least squares methods use optimization algorithms that are especially designed for the case where the *objective function* is a sum of the squares – often of differences between observed and predicted values.

Bayesian Calibration. This method is based on Bayes Theorem and uses a likelihood function.

# 2.3. Parameter Studies and Sensitivity Analysis

In DAKOTA, a parameter study consists of computing response data sets at a selection of points in the parameter space. DAKOTA offers four parameter study methods:

- *Vector* = evaluate the RF at points along a straight line in parameter space.
- *List* = evaluate the RF at an arbitrary set of user-specified points.
- *Centered* = evaluate the RF at a cross-like set of points near a specified point.
- *Multidimensional* = evaluate the RF at a lattice of evenly-spaced points.

Here, RF is used as an abbreviation for *response function* (which need not be an objective function) and the word *points* refers to points in the multidimensional (design) parameter space. The values in response data sets (of the response function) can be examined by the user, visualized using line graphs or other plots, or provided as input to subsequent analysis routines.

#### 2.4. Uncertainty Quantification

The expression "uncertainty quantification" usually refers to the specific process of studying how uncertainties in input variables are forward propagated through a computational model to produce uncertainties in output (or response) variables. Methods for doing this are also called "nondeterministic analysis methods".

Input Variables with Aleatoric Uncertainty. If an input variable is viewed as having aleatoric uncertainty, it is assumed that there is sufficient information to assign a probability distribution to the uncertainty. DAKOTA supports most of the well-known probability distributions. In this case, a variety of methods can be used to estimate the probability distributions (or at least statistics such as mean, standard deviation, coefficients of variation and 95% confidence intervals) of the output (or response) variables that result from forward propagation of input errors through the model.

Input Variables with Epistemic Uncertainty. If an input variable is viewed as having epistemic uncertainty, it is generally assumed that there is not enough information to assign a probability distribution to the uncertainty. In this case, various types of *interval analysis* are used which assume only that the input variable lies in a particular range of values or interval. Such methods then compute analogous intervals for the output variables that result from forward propagation of input errors through the model.

DAKOTA contains a variety of methods intended for the case where input variables have aleatoric uncertainty, as well as other methods intended for the case where they are subject to epistemic uncertainty. DAKOTA also has the ability to analyze cases where the input variables have a mixture of aleatoric and epistemic uncertainty (e.g. a nested Dempster-Shafer evidence theory approach.) Many of these methods also support the case where multiple input variables are correlated.

#### 2.5. Propagation of Errors (or Uncertainty)

This may be thought of as a simpler and more tractable special case that falls under the heading of Uncertainty Quantification. The term "propagation of errors" refers to methods for computing or estimating the error associated with variables that are computed as functions of other variables, assuming that the errors associated with the original variables are known. In other words, the errors associated with the quantity f(V) are computed in terms of the errors associated with V. (Is it assumed that the errors of the original variables come from a Gaussian distribution?) The book by Taylor (1982) provides error formulas for many common functions of one or more variables. The Wikipedia article titled "Propagation of Uncertainty" also provides a table of such error formulas. In these formulas, error is typically quantified in terms of standard deviations or covariances. However, for the typical case where f(V) is nonlinear, the formulas use truncated series expansions and therefore tend to be biased.

There is also a standard procedure (or formula) in probability theory that allows the distribution of a function of a random variable to be computed when the distribution of the random variable itself is known. The formula is valid for arbitrary probability density functions (pdfs); the original random variable doesn't need to come from a Gaussian or normal distribution. When applicable, this formula provides a more precise method for computing propagation of errors. See Ross (2001).

#### 2.6. Design of Computer Experiments

The expression "design of computer experiments" refers to a collection of methods that have the primary purpose of extracting as much information as possible (e.g. trend data) from a problem's parameter space using only a limited number of *sample points*. Some methods focus on sample points that are at the extremes of the parameter space, such as: Central Composite Design, Box-Behnken Design, Full Factorial Design and Fractional Factorial Design, as a means of identifying trends. Other methods use a collection of sample points that are "space-filling", with good coverage of the entire parameter space, such as: Orthogonal Array Designs, Latin Hypercube Sampling, Monte Calo Sampling and Quasi Monte Carlo Sampling. DAKOTA offers a variety of different methods for this type of analysis, including:

DDACE = Distributed Design and Analysis of Computer Experiments

- Central Composite Design (CCD, i.e. Box-Wilson)
- Box-Behnken Design
- Orthogonal Array (OA) Designs
- Grid Design
- Monte Carlo Design
- Latin Hypercube Sampling (LHS) Design
- OA-LHS Design (hybrid of OA and LHS above)

#### FSUDace

- Halton Quasi-Monte Carlo Sampling
- Hammersley Quasi-Monte Carlo Sampling
- Centroidal Voronoi Tessellation (CVT)

#### PSUADE MOAT

See the DAKOTA documentation for detailed discussions of these methods.

#### 2.7. Other Important Concepts

There are many other important concepts in the realm of uncertainty quantification that are beyond the scope of this document. Since detailed discussions can easily be found online (e.g. see the section called Direct Links to Wikipedia Articles below), here we simply list some of the most important ones.

- Accuracy vs. Precision
- Aleatoric (Statistical) vs. Epistemic (Systematic) Uncertainty
- Data assimilation
- Decision theory
- Equifinality (Beven, 2001, 2006)
- Estimation theory
- Fuzzy logic
- Lesson of Geocentric (Ptolemaic) vs. Heliocentric (Copernican) models
- Parametric vs. Non-parametric (or Distribution-free) methods
- Response surface methodology
- Risk, reliability and failure analysis

# 3. Quantification of Model Uncertainty

#### 3.1. Sources of Uncertainty in Models

There are many possible sources of uncertainty in models. Any of them, taken alone or in combinations, can be the underlying reason why a computational model fails to make accurate predictions for variables of interest. These sources of uncertainty can be classified into three main categories, namely (1) model inadequacy, (2) input data inadequacy and (3) user errors. Note that even if the mathematics and physics of a model were perfect, perfect predictions would not be possible because input data (e.g. initial conditions over the model domain) will always be imperfectly known and incomplete. For spatial models, surrogates for actual measurements across the model domain based on remotely sensed imagery are often the best available data for initial conditions (e.g. soil moisture or rainfall rates). The following subsections provide key examples for each of the three main sources of model uncertainty.

#### Model Inadequacy

- Lack of knowledge of the true, underlying physics (e.g. precession of Mercury)
- Neglected effects or simplifying assumptions (e.g. air resistance)
- Incorrect implementation or *developer error* (e.g. bugs)
  - o Regressions (bugs due to updates or improvements)
  - o Bugs may be in software dependencies or in model itself.
  - Mismatched units (and failure to convert)
  - o Problems at domain boundaries
- Numerical method and approximation problems (convergence, stability, consistency, fidelity, etc.)
- Calibration problems
- Model coupling problems (e.g. feedbacks, conservation problems)

#### Input Data Inadequacy

- Poor spatial or temporal resolution
- Poor quality
- Measurement or observation error (aleatoric uncertainty)
- Storage or transfer errors (e.g. byte order, data type, truncated files, formatting, etc.)

### User Errors

- Preparation of input data (model setup)
- Incorrect or unintended use (e.g. unawareness of limitations)

A "bias" can be viewed as a possible characteristic or property of model error or uncertainty. This is the tendency to consistently over- or under-predict and may be due to a neglected effect (e.g. air resistance), an approximation that takes the form of an inequality, the numerical method used to solve a differential equation, or many other causes.

### 3.2. Ways to Address Uncertainty in Models

*Model Inadequacy*. Scientific research to better understand physical processes and systems that are poorly understood and various forms of testing are the main ways that uncertainty due to model inadequacy can be reduced. In terms of testing, there are five main things that models can be tested or evaluated against in order to reduce uncertainty due to *model inadequacy* namely:

- Analytic solutions and test problems
- Measured data (i.e. observed vs. predicted)
- Valid range or reasonableness (e.g. sanity tests)
- Other models (especially for complex models, e.g. climate models)
- Their former selves (e.g. regression and unit tests, often automated)

Models tend to become more reliable and robust when they are used by large groups of people, particularly when their source code is open.

*Input Data Inadequacy.* The methods of Uncertainty Quantification and Propagation of Error (as discussed in the Background section) provide the primary tools for assessing this source of uncertainty. Better data collection methodologies and careful data preparation and documentation (with provenance metadata) are two of the main ways that uncertainty due to input data inadequacy can be reduced. As with models, data sets tend to become more reliable and robust when they are used by large groups of people.

User Errors. User errors can be addressed in a variety of ways, including:

- Documentation (e.g. tech tips, FAQs, manuals, tutorials, context help)
- GUIs (that can restrict possible inputs based on context)
- Software to check inputs, conditions, compatibility, etc.
- Training (and certification)
- Supervision by an expert

A "checklist" approach can be used to completely eliminate some sources of error. Checklists help to ensure consistency and completeness in carrying out a complex task. They can be used within software, by a developer or by a user. Well-known examples of checklists that are used to reduce uncertainty (and improve safety and reliability) include:

- pilot's pre-flight checklist
- motorcyclist pre-ride checklist
- surgical safety checklist (developed by Dr. Atul Gawande for World Health Organization.)
- industrial procedure checklists

#### 4. Software for Uncertainty Analysis

There are a vast number of software packages for uncertainty analysis that can be found using a simple web search. A few notable examples are:

DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) http://dakota.sandia.gov/index.html

Jupiter API (Joint Universal Parameter IdenTification and Evaluation of Reliability) http://water.usgs.gov/software/JupiterApi/ Python Packages: uncertainty, soerp, mcerp http://pythonhosted.org/uncertainties/

The intent is for this section to be expanded in a future version of this document. The remainder of this document will focus on the DAKOTA package.

#### 5. Overview of DAKOTA 5.1. What is DAKOTA?

DAKOTA is an acronym that stands for Design Analysis Kit for Optimization and Terascale Applications. The DAKOTA project started in 1994 as a toolbox of optimization methods and over time has accumulated a broad variety of gradient-based and nongradient-based optimizers from many different "vendor packages" including: DOT, NPSOL, NLPQL, CONMIN, OPT++, APPS, SCOLIB, NCSU, and JEGA. However, DAKOTA is now much more than an optimization toolkit and includes methods for global sensitivity and variance analysis, parameter estimation, uncertainty quantification, verification, surrogate-based optimization, hybrid optimization and optimization under uncertainty. A key advantage of DAKOTA is that it provides "umbrella" access to the algorithms in many different vendor packages through a common user interface, namely the DAKOTA input file. DAKOTA was designed to be extensible and its capabilities are growing continuously as new vendor packages are brought under the umbrella and as new methods are added by the DAKOTA team. Other big advantages of DAKOTA are that it supports parallel computation for all of its algorithms and it is released under a GNU LGPL open-source license (as of version 5).

The DAKOTA 5.3.1 documentation is vast and includes a 327-page User's Manual, a 229-page Reference Manual, a 77-page Theory Manual and a 1013-page Developer's Manual. These manuals are filled with technical terminology and acronyms that can make them difficult to read. They are all available at: <a href="http://dakota.sandia.gov/index.html">http://dakota.sandia.gov/index.html</a>. One of the goals of this report is to distill essential information from these manuals into a form that is more readily accessible to CSDMS software engineers and to modelers, especially those who are not experts in uncertainty quantification but are interested in how DAKOTA can help them understand and quantify the uncertainty in their models.

#### 5.2. What Can DAKOTA Do?

A good way to learn some of the key terminology used by DAKOTA and to get an overview of what DAKOTA has to offer modelers is to discuss the six blocks that are found in a DAKOTA Input File.

The **strategy** keyword marks the beginning of the *strategy block* in a DAKOTA Input File. This block is used to specify the overall, top-level *solution strategy* that DAKOTA is to use for solving the problem of interest. The "strategy selection" must be one of the following:

- **single\_method** = use a single method (i.e. algorithm, see next paragraph) to obtain results (e.g. to seek an optimal design). This is the default and most commonly used option.
- **hybrid** = use multiple methods (i.e. algorithms, see next paragraph) to seek an optimal design. The manner in which the methods can be combined may be *collaborative, embedded* or *sequential*.
- **multi\_start** = use a single method to seek an optimal design, but start the simulation model multiple times, typically on different processors and with different initial values for the design variables.
- **pareto\_set** = use different weightings with multiple objective functions to seek a *set of optimal designs* (a so-called Pareto set) that balance tradeoffs between competing design objectives. This also requires starting the simulation model multiple times, typically on different processors.

The **method** keyword marks the beginning of the *method block* in a DAKOTA input file. This block specifies the type of analysis that DAKOTA is to perform, or the specific algorithm that DAKOTA is to use for solving a given problem. DAKOTA includes many methods for optimization, uncertainty quantification, least squares, design of experiments, and parameter studies. Method names are often prefixed with a string that indicates the third-party "vendor package" or library that provides the method. An overview of the many available methods in DAKOTA is given in a subsequent section called: Overview of Libraries and Methods Available in DAKOTA.

The **model** keyword marks the beginning of the *model block* in a DAKOTA input file. This block specifies a *model type*, or a specification for how variables (input) are to be mapped to responses (output). The "model selection" must be one of the following:

- **single** = use a single interface to map variables into responses. This is the most common model selection.
- **surrogate** = use an approximation to a "truth" model --- which can be *global, multipoint, local* or *hierarchical* -- to map variables to responses. This can be far less computationally costly than using the original model. For the *global surrogate* option an approximation type is chosen from: *polynomial, gaussian\_process, neural\_network, mars, moving least squares, radial\_basis.*
- **nested** = use nested models (i.e. model and submodel, with inner and outer loops) to map variables to responses. For this option the inner loop computes some responses and the outer loop computes responses from those responses. For example, the inner loop may iterate to compute some values and then the outer loop computes statistics such as mean or median from those values.

The **variables** keyword marks the beginning of the *variables block* in a DAKOTA input file. This block is used to specify the parameters that are to be iterated by a particular method, which can include *design*, *state* and *uncertain* variables. Design variables are those that an optimizer adjusts in order to find an optimal design. State variables are any non-design variables that are mapped through the simulation interface. All variables may be either continuous or discrete.

The **interface** keyword marks the beginning of the *interface block* in a DAKOTA input file. This block is used to specify the type of interface that DAKOTA is to use for interacting with a simulation model that maps variables (input) to responses (output). The "interface selection" must be one of the following:

- fork = start simulations by calling an external executable, as specified with the *analysis\_drivers* keyword. DAKOTA uses "fork calls" to create separate Unix processes for executions of the user-supplied executable. Communication between DAKOTA and the simulation model is through file I/O, using a specified *parameters\_file* for input and a *results\_file* for output, and using specified scripts to transfer values from the *parameters\_file* to the model's configuration file and from the model's output files to the *results\_file*. This is the default and most commonly used option.
- **system** = virtually the same as the fork option, but using a direct system call. Users are strongly encouraged to use the fork option instead whenever possible. It is still included for portability and backward compatibility.
- **direct** = start simulations using direct calls to functions (e.g. simulations and tests) that have been compiled and linked into DAKOTA. This option avoids the file I/O overhead of the fork option but requires more work to set up.
- **python** = start simulations using a library-linked interface to Python. This option allows DAKOTA to make function evaluation calls directly to an analysis function in a user-provided Python module. Data is passed using multiply-subscripted lists. DAKOTA functions are not callable from the Python code, however.
- **numpy** = the same as the python option, except that data is passed using NumPy arrays.
- **matlab** = start simulations using a library-linked interface to Matlab
- **scilab** = start simulations using a library-linked interface to Scilab

• grid = start simulations across different computer resources using computational grid services such as Condor and Globus (experimental and not operational in DAKOTA 5.3.1).

The **responses** keyword marks the beginning of the *responses block* in a DAKOTA input file. This block is used to specify the set of "output variables" that are to be returned through the interface as the result of a "function evaluation" in the simulation model on the "variables" (input variables).

# 5.3. Connecting DAKOTA to a Model Using the "fork" Interface Option

This is a "loose coupling" option where all communication between DAKOTA and a simulation model is through file I/O. It is also the default. DAKOTA refers to its configuration file (as the term is used by CSDMS) as the DAKOTA Input File. With the "fork" interface option, DAKOTA uses two other intermediary files to help it communicate with the model called the DAKOTA Parameters File and DAKOTA Results File. DAKOTA writes parameters that it wants to set into the model into the DAKOTA Parameters File. Two different formats for this file are supported, as specified using keywords (e.g. *aprepro*) in the *interface block* of the DAKOTA Input File. DAKOTA reads results that it requires from a model run from the DAKOTA Parameters file. Similarly, a data post-processing script is required to create a valid DAKOTA Results File from the Model Output File(s). The names of these scripts can be specified with the *input\_filter* keywords in the *interface block* of a DAKOTA Input File.

**DAKOTA Input (or Configuration) File.** This is the file that DAKOTA reads to configure itself each time it runs. Its name will typically be something like: "dakota\_<model\_name>.in". It specifies the study that the user wants DAKOTA to perform along with all of the settings required for that study. The structure of a DAKOTA input file is described in a subsequent section called Basic Template of a DAKOTA Input File. The "fork" interface option (and its associated settings) are specified in the *interface block* of the DAKOTA input file by setting the *interface selection* to **fork**.

**Note:** CSDMS could possibly use its WMT GUI to help users create DAKOTA Input Files. However, this will not be possible with simple, tabbed dialogs due to the multitude of different analysis methods that can be selected, each with its own set of parameters. Something like a wizard-style GUI would probably be needed.

**DAKOTA Parameters File.** This file has one of two possible formats (dprepro and aprepro) and contains parameters (design variables) that DAKOTA wants the model to use the next time it runs. The name of this file is specified with the *parameters\_file* keyword in the *interface block* of the DAKOTA Input File. The default name is "params.in".

**DAKOTA Results File**. This file has a particular format and contains a block of requested data values, a block of requested gradients (first derivatives) and a block of requested Hessians (second derivatives), for each response variable. The name of this file is specified with the *results\_file* keyword in the *interface block* of the DAKOTA Input File. The default name is "results.out".

**Model Executable.** The name of the model executable is specified with the *analysis\_drivers* keyword in the *interface block* of the DAKOTA Input File. Depending on the DAKOTA methods that are used for a particular study (as specified in the DAKOTA Input File), DAKOTA may call the model's executable once or multiple times. Before each call to the model's executable, a new model configuration file with the parameter (design variable) settings that are required for that model run must be created using one of the two mechanisms described in the next paragraph.

**Model Input (or Configuration) File.** This is the configuration file that a model reads before it runs to configure its adjustable parameters. Given a template of a model's configuration file (with placeholders for valid configuration parameters), DAKOTA can optionally use its built-in DPrePro Perl script to transfer parameters from a DAKOTA Parameters File into a new model configuration file. The model input file

template can be specified with the *template\_files* and *template\_directory* keywords in the *interface block* of the DAKOTA Input File. Alternately, the name of an executable script that DAKOTA should call to create a Model Input File from a DAKOTA Parameters file can be specified with the *input\_filter* keyword in the *interface block* of the DAKOTA Input File.

**Model Output File(s).** These are whatever output files a model creates to save the results of a model run. DAKOTA needs values from these files to be transferred into a valid DAKOTA Results File. The name of an executable script that DAKOTA should call to create a DAKOTA Results file from the Model Output File(s) can be specified with the *output\_filter* keyword in the *interface block* of the DAKOTA Input File. **Note:** The script specified by *output\_filter* could also be used to compute gradients and hessians (as needed by gradient-based optimization methods) if the model is unable to provide them. **Note:** Each model will likely require its own *output\_filter* script.

# 5.4. Connecting DAKOTA to a Model Using the "direct" Interface Option

This is a "tight coupling" option where all communication between DAKOTA and a simulation model is through direct function calls. This option and its associated settings are specified in the *interface block* of the DAKOTA input file by setting the *interface selection* to **direct**. For this option, the *analysis\_driver* keyword is set to the name of the (now internal to DAKOTA) function that is to be called.

**Note:** DAKOTA could use BMI setter functions to set values directly into a BMI-enabled model component.

# 5.5. Connecting DAKOTA to a Model Using the "python" Interface Option

DAKOTA also supports a library-linked interface to Python (as well as Matlab and Scilab). This option allows DAKOTA to make function evaluation calls directly to an analysis function in a user-provided Python module. With the "python" interface option, data is passed to the module using multiply-subscripted lists. With the "numpy" interface option, data is passed to the module using NumPy arrays. This does not make DAKOTA functions callable from the Python code, however. For that, see the next section.

Since the CMI interface for most CSDMS model components is provided with a Python wrapper around a BMI-enabled model, this interface option, combined with using DAKOTA as a library (see the next section) may provide a good strategy for integrating DAKOTA with the CSDMS modeling framework.

#### 5.6. Interfacing with DAKOTA as a Library

The DAKOTA toolkit can be linked into another application for use as an algorithm library as explained in Chapter 5 of the DAKOTA 5.3.1 Developer's Manual. This allows the other application (e.g. a model) to make calls to DAKOTA. As explained in the manual, however:

"The use of Dakota as an algorithm library should be distinguished from the linking of simulations within Dakota using the direct application interface. In the former, Dakota is providing algorithm services to another software application, and in the latter, a linked simulation is providing analysis services to Dakota. It is not uncommon for these two capabilities to be used in combination, where a simulation framework provides both the "front end" and the "back end" for Dakota."

# 5.7. Launching DAKOTA

Send standard output (stdout) and standard error (stderr) messages to the terminal: % dakota –i dakota.in

Send standard output (stdout) and standard error (stderr) messages to named files:

% dakota -- i dakota.in -- o dakota.out -- e dakota.err

#### 5.8. Overview of Libraries and Methods Available in DAKOTA

This section provides an overview of all the third-party libraries and methods that are available in DAKOTA. The available methods are organized first by their type, and then by the library or vendor package that provides them. The keyword DAKOTA uses to identify each method is listed, along with a short description of the method. Sometimes different implementations of the same method (e.g. Sequential Quadratic Programming method) are available from multiple vendors/libraries, and each may have unique characteristics specific to that implementation. Each method typically has its own set of "method-dependent controls" or control parameters. More complete descriptions of these methods and their specific control parameters can be found in the indicated section of the DAKOTA 5.3.1 Reference Manual.

#### **Optimization** Methods (4.4)

DOT Library (Version 4.20): Vanderplaats Research and Development (1995)

dot\_bfgs = Broyden-Fletcher-Goldfarb-Shanno method

dot\_frcg = Fletcher-Reeves Conjugate Gradient methods for unconstrained optimization

dot\_mmfd = Modified Method of Feasible Directions method

dot\_slp = Sequential Linear Programming method

dot\_sqp = Sequential Quadratic Programming method

#### NPSOL Library (Version 4.0): Gill et al. (1986)

npsol\_sqp = Sequential Quadratic Programming, nonlinear programming optimizer for constrained minimization.

#### NLPQL Library: Schittkowski (2004)

nlpql\_sqp method: Sequential Quadratic Programming, nonlinear programming optimizer for constrained minimization.

#### CONMIN Library: Vanderplaats (1973) (public domain)

conmin\_frcg = Fletcher-Reeves Conjugate Gradient methods for unconstrained optimization conmin\_mfd = Method of Feasible Directions for constrained optimization.

OPT++ Library: Meza et al. (2007)

optpp\_cg = Polak-Ribiere Conjugate Gradient method (unconstrained) optpp\_q\_newton = Quasi-Newton method optpp\_fd\_newton = Finite-Difference Newton method optpp\_newton = full Newton method optpp\_pds = Parallel Direct Search method (with bound constraints)

APPS or HOPSPACK Library: Gray and Kolda (2006), Plantenga (2009) asynch\_pattern\_search = Asynchronous Parallel Pattern Search method

## SCOLIB Library (formerly known as COLINY): https://software.sandia.gov/trac/acro coliny\_cobyla = Constrained Optimization BY Linear Approximations (COBYLA) method (extension to the Nelder-Mead simplex algorithm) coliny\_direct = Dividing RECTangles (DIRECT), derivative-free, global optimization method coliny\_ea = Evolutionary Algorithm (EA) method coliny\_pattern\_search = Pattern Search method coliny\_solis\_wets = Solis-Wets algorithm, simple greedy local search method

NCSU Library (North Carolina State University): Gablonsky (2001) ncsu\_direct = Dividing RECTangles (DIRECT), derivative-free, global optimization method

JEGA Library: Eddy and Lewis (2001)

moga = Multi-Objective Genetic Algorithm (MOGA), via Pareto optimization soga = Single-Objective Genetic Algorithm (SOGA), single objective function

NOMAD Library:

mesh\_adaptive\_search = Mesh Adaptive Search

*Note:* The libraries or "vendor packages" (or "iterator packages") which can compute their own gradients are: DOT, CONMIN, NPSOL, NL2SOL, NLSSOL and OPT++.

# Least Squares Methods (4.5)

#### DAKOTA:

nl2sol = Nonlinear Least Squares via adaptive, trust region method nlssol = Nonlinear Least Squares via adaptive, trust region method2

#### OPT++ Library: Meza et al. (2007)

optpp\_g\_newton = Gauss-Newton method (for unconstrained, bound-constrained or generallyconstrained problems)

#### Surrogate-Based Minimization Methods (4.6)

surrogate\_based\_local = Surrogate-Based Local method
surrogate\_based\_global = Surrogate-Based Global method
efficient\_global = Efficient Global method

#### Uncertainty Quantification Methods (4.7)

DAKOTA Aleatory Uncertainty Quantification Methods:

sampling = Nondeterministic sampling method (random or Latin Hypercube) (4.7.1.1)
local\_reliability = Local reliability methods (4.7.1.2)
global\_reliability = Global reliability methods (4.7.1.3)
importance\_sampling = Importance Sampling methods (4.7.1.4)
adaptive\_sampling = Adaptive Sampling methods (4.7.1.5)
polynomial\_chaos = Polynomial Chaos method (4.7.1.6)
stoch\_collocation = Stochastic Collocation method (4.7.1.7)

DAKOTA Epistemic Uncertainty Quantification Methods:

local\_interval\_est = Local Interval Estimation (4.7.2.1) global\_interval\_est = Global Interval Estimation (4.7.2.2) local\_evidence = Local Evidence Theory (Dempster-Shafer) methods (4.7.2.3) global\_evidence = Global Evidence Theory (Dempster-Shafer) methods (4.7.2.4)

#### Nondeterministic Calibration Methods (4.8)

bayes\_calibration queso = Bayesian Calibration via QUESO library (UT Austin) bayes\_calibration gpmsa = Bayesian Calibration via GPMSA library (LANL)

# Solution Verification Methods (4.9)

richardson\_extrap = Richardson Extrapolation method (4.9.1)

# Design of Computer Experiments Methods (4.10)

DDACE Library (Distributed DACE) (4.10.1):

dace = Design and Analysis of Computer Experiments (DACE)

FSUDace Library (Florida State University) (4.10.2):

fsu\_quasi\_mc = quasi-Monte Carlo sampling, based on Halton or Hammersley sequence fsu\_cvt = Centroidal Voronoi Tessellation

PSUADE Library (Problem Solving Environment for Uncertainty Analysis and Design Exploration): psuade\_moat = PSUADE Morris One-At-A-Time (MOAT) method (4.10.3)

#### Parameter Study Methods (4.11)

DAKOTA Parameter Study Methods (ParamStudy class): vector\_parameter\_study = Vector Parameter Study method (4.11.1) list\_parameter\_study = List Parameter Study method (4.11.2) centered\_parameter\_study = Centered Parameter Study method (4.11.3) multidim\_parameter\_study = Multidimensional Parameter Study method (4.11.4)

#### 5.9. Basic Template for a DAKOTA Input File

DAKOTA Input Files are described in detail in Chapter 10 of the DAKOTA 5.1 Reference Manual. A DAKOTA input file is composed of six blocks that specify the *strategy, method, model, variables, interface* and *responses* that are to be used for a given DAKOTA run. (If a block is omitted then default settings may be used.) Within each block a selection is made and then additional controls that are either independent of or dependent on that selection are specified. A complete listing of all supported options/controls requires 30 pages. However, a DAKOTA input file is always constructed according to the following basic template.

#### strategy,

<strategy independent controls> <strategy selection> <strategy dependent controls>

"strategy selection" must be in: hybrid, multi\_start, pareto\_set, single\_method

#### method,

<method independent controls> <method selection> <method dependent controls>

"method selection" must be in:

#### Optimization methods:

asynch\_pattern\_search, coliny\_cobyla, coliny\_direct, coliny\_pattern\_search, coliny\_solis\_wets, coliny\_ea, conmin\_frcg, conmin\_mfd, dot\_frcg, dot\_mmfd, dot\_bfgs, dot\_slp, dot\_sqp, ncsu\_direct, nlpql\_sqp, npsol\_sqp, optpp\_cg, optpp\_fd\_newton, optpp\_newton, optpp\_pds, optpp\_q\_newton, moga, soga, *Least Squares methods:* nl2sol, nlssol\_sqp, optpp\_g\_newton, *Surrogate-Based Minimization methods:* surrogate\_based\_local, surrogate\_based\_global, efficient\_global, *Uncertainty Quantification methods:* 

sampling, local\_reliability, global\_reliability, importance\_sampling, adaptive\_sampling, polynomial\_chaos, , stoch\_collocation, local\_interval\_est, global\_interval\_est, local\_evidence, global\_evidence

Nondeterministic Calibration methods: bayes\_calibration (queso or gpmsa option) Solution Verification methods: richardson\_extrap Design of Computer Experiments methods: dace, fsu\_quasi\_mc, fsu\_cvt, psuade\_moat, Parameter Study methods: vector\_parameter\_study, list\_parameter\_study, centered\_parameter\_study, multidim\_parameter\_study Other methods: nonlinear\_cg, dl\_solver

#### model,

<model independent controls> <model selection> <model dependent controls>

"model selection" must be in: single, surrogate, nested If "surrogate", choose a type from: global, multipoint, local, hierarchical If "global surrogate", choose an "approximation type" from: polynomial, gaussian\_process, neural\_network, mars, moving least squares, radial\_basis

#### variables,

<set identifier> <active variable specification> <variable domain specification> <continuous design variables specification> <discrete design range variables specification> <discrete design set integer variables specification> <discrete design set real variables specification> <normal uncertain variables specification> <lognormal uncertain variables specification> <uniform uncertain variables specification> <loguniform uncertain variables specification> <triangular uncertain variables specification> <exponential uncertain variables specification> <br/>
<br/>
deta uncertain variables specification> <gamma uncertain variables specification> <gumbel uncertain variables specification> <frechet uncertain variables specification> <weibull uncertain variables specification> <histogram bin uncertain variables specification> <poisson uncertain variables specification> <br/>
<br/>
dinomial uncertain variables specification> <negative binomial uncertain variables specification> <geometric uncertain variables specification> <hypergeometric uncertain variables specification> <histogram point uncertain variables specification> <uncertain correlation specification> <continuous interval uncertain variables specification> <discrete interval uncertain range variables specification>

<discrete uncertain set integer variables specification> <discrete uncertain set real variables specification> <continuous state variables specification> <discrete state range variables specification> <discrete state set integer variables specification> <discrete state set real variables specification>

#### interface,

<interface independent controls> <algebraic mappings specification> <simulation interface selection> <simulation interface dependent controls>

"interface selection" must be in: fork, system, direct, python, numpy, matlab, scilab, grid

#### responses,

<set identifier> <response descriptors> <function specification> <gradient specification> <Hessian specification>

#### 5.10. DAKOTA Acronyms

```
AMV = Advanced Mean Value
ANN = Artificial Neural Network
ANOVA = Analysis of Variance
ASV = Active Set Vector
APPS = Asynchronous Parallel Pattern Search
BPA = Basic Probability Assignment
CBF = Cumulative Belief Function
CCDF = Complementary CDF
CDF = Cumulative Distribution Function
CDV = Continuous Design Variables
CG = Conjugate Gradient
COBYLA = Constrained Optimization BY Linear Approximations
COLINY = (now SCOLIB) #####
CONMIN = ######
CPF = Cumulative Plausibility Function
DACE = Design and Analysis of Computer Experiments
DDCASE = Distributed DACE
DDISV = Discrete Design Integer Set Variables
DIRECT = DIviding RECTangles (algorithm)
DoE = Design of Experiments
DOT = #######
DRAM = Delayed Rejection and Adaptive Metropolis
DREAM = DiffeRential Evolution Adaptive Metropolis
DVV = Derivative Variables Vector
EA = Evolutionary Algorithm
EGO = Efficient Global Optimization
EIF = Expected Improvement Function
```

FRCG = Fletcher-Reeves Conjugate Gradient FSU = Florida State University (e.g. FSU-DACE) GP = Gaussian Process JEGA = John Eddy Genetic Algorithm (see MOGA, SOGA) LHS = Latin Hypercube Sampling LLNL = Lawrence Livermore National Lab LS = Least Squares MARS = Multivariate Adaptive Regression Splines MCMC = Markov Chain Monte Carlo MFD = Method of Feasible Directions MLS = Moving Least Squares MMFD = Modified Method of Feasible Directions MOAT = Morris One-At-a-Time (psuade\_moat method) MOGA = Multi-Objective Genetic Algorithm (see SOGA, JEGA) MPP = Most Probable Point MV = Mean Value (method, also known as MVFOSM) NCSU = North Carolina State University NLPQL = ######### NLS = Nonlinear Least Squares PCE = Polynomial Chaos Expansion PDF = Probability Density Function PDS = Parallel Direct Search PMA = Performance Measure Approach PSUADE = Problem Solving environment for Uncertainty Analysis and Design Exploration QOI = Quantities of Interest QUESO = Quantification of Uncertainty for Estimation, Simulation and Optimization RBF = Radial Basis Functions RIA = Reliability Index Approach RNG = Random Number Generator SBO = Surrogate-Based Optimization SBONLS = SBO Nonlinear Least Squares SE = Stochastic Expansion SLP = Sequential Linear Programming (see SQP) SNLL = Sandia National Laboratories - Livermore SOGA = Single Objective Genetic Algorithm (see JEGA, MOGA) SQP = Sequential Quadratic Programming (see SLP) TANA = Two-point Adaptive Nonlinear Approximation

#### 6. Conclusions and Recommendations

A gentle introduction to a large number of topics that fall within the purview of uncertainty quantification and closely related subjects was provided in section 2. A basic understanding of these concepts is essential in order to understand and appreciate the wide variety of capabilities that are available within the DAKOTA software package. It is easy for the uninitiated to become lost due to all of the new concepts and technical terminology, some of which is used with a different meaning in other disciplines.

In section 3.1 it was argued that the primary sources of model uncertainty can be usefully organized into three groups, namely: *model inadequacy, input data inadequacy* and *user errors.* Specific ways to reduce these various types of uncertainty were then discussed in section 3.2.

An overview of DAKOTA was provided in section 5. This overview provided sufficient detail for readers to quickly begin using DAKOTA, and to make better use of DAKOTA's documentation, even if initially unfamiliar with many of the underlying concepts and methods. It explained in a fair amount of concise detail the various ways in which DAKOTA can be connected to a model. Section 5 (and also section 2) also identified what are expected to be the key technical issues with regard to integrating DAKOTA with CSDMS.

One of these is concerned with how to create a service component that can compute the derivatives required for DAKOTA methods that require derivatives. It is not entirely clear whether this can be done entirely outside of a model's own source code or whether extensions to the Basic Model Interface (BMI) will be necessary, especially if the goal is to provide *automatic differentiation*, as defined in section 2. More work will be needed to design an approach to this problem that requires minimal work on the part of developers without imposing a significant extra computational cost. It should also be noted that while the tools in packages like DAKOTA help users to quantify, assess and understand the uncertainty in models, they do not automatically or necessarily lead to any *reduction* in a model's uncertainty.

Finally, as discussed in the Introduction, there are significant social, cultural and educational barriers that must be overcome in order for the modeling community served by CSDMS to begin incorporating uncertainty quantification methods into their workflow. While the inverse modeling community already has an appreciation for these methods, this is much less the case for the forward modeling community. Clinics and training workshops may be one way to educate, excite and encourage this modeling community to begin using these methods once they are made available within the CSDMS modeling framework.

#### Appendix A. Direct Links to Wikipedia Articles

http://en.wikipedia.org/wiki/Accuracy\_and\_precision http://en.wikipedia.org/wiki/Adjoint\_equation http://en.wikipedia.org/wiki/Ant\_colony\_optimization\_algorithms http://en.wikipedia.org/wiki/Artificial\_bee\_colony\_algorithm http://en.wikipedia.org/wiki/Automatic differentiation http://en.wikipedia.org/wiki/Biogeography-based\_optimization http://en.wikipedia.org/wiki/Checklist http://en.wikipedia.org/wiki/COBYLA http://en.wikipedia.org/wiki/Computer experiment http://en.wikipedia.org/wiki/Conjugate\_gradient\_method http://en.wikipedia.org/wiki/Cuckoo\_search http://en.wikipedia.org/wiki/DAKOTA http://en.wikipedia.org/wiki/Derivative-free\_optimization http://en.wikipedia.org/wiki/Design\_of\_experiments http://en.wikipedia.org/wiki/Differential\_evolution http://en.wikipedia.org/wiki/Eight\_queens\_puzzle (compare to Latin square) http://en.wikipedia.org/wiki/Equifinality http://en.wikipedia.org/wiki/Estimation\_theory http://en.wikipedia.org/wiki/Evolutionary\_algorithm http://en.wikipedia.org/wiki/Experimental\_uncertainty\_analysis http://en.wikipedia.org/wiki/Factor analysis http://en.wikipedia.org/wiki/Genetic\_algorithm http://en.wikipedia.org/wiki/Global\_optimization http://en.wikipedia.org/wiki/GLUE\_(uncertainty\_assessment) http://en.wikipedia.org/wiki/Gradient descent http://en.wikipedia.org/wiki/Hessian\_matrix http://en.wikipedia.org/wiki/Intelligent\_Water\_Drops\_algorithm http://en.wikipedia.org/wiki/Jacobian\_matrix http://en.wikipedia.org/wiki/Known\_unknowns http://en.wikipedia.org/wiki/Latin\_hypercube\_sampling http://en.wikipedia.org/wiki/Latin\_square http://en.wikipedia.org/wiki/Least\_squares http://en.wikipedia.org/wiki/Line search http://en.wikipedia.org/wiki/Linear\_programming http://en.wikipedia.org/wiki/List\_of\_optimization\_software

http://en.wikipedia.org/wiki/Loss\_function http://en.wikipedia.org/wiki/Mathematical optimization http://en.wikipedia.org/wiki/Memetic algorithm http://en.wikipedia.org/wiki/Metaheuristic http://en.wikipedia.org/wiki/Nelder-Mead\_method http://en.wikipedia.org/wiki/Newton%27s method in optimization http://en.wikipedia.org/wiki/Non-linear\_least\_squares http://en.wikipedia.org/wiki/Nonlinear\_programming http://en.wikipedia.org/wiki/Numerical\_differentiation http://en.wikipedia.org/wiki/Optimal design http://en.wikipedia.org/wiki/Pareto\_efficiency http://en.wikipedia.org/wiki/Particle swarm optimization http://en.wikipedia.org/wiki/Pattern search (optimization) http://en.wikipedia.org/wiki/Polynomial chaos http://en.wikipedia.org/wiki/Principal\_component\_analysis http://en.wikipedia.org/wiki/Propagation of uncertainty http://en.wikipedia.org/wiki/Quantification\_of\_margins\_and\_uncertainties http://en.wikipedia.org/wiki/Quasi-Newton method http://en.wikipedia.org/wiki/Random\_search http://en.wikipedia.org/wiki/Regression\_testing http://en.wikipedia.org/wiki/Response\_surface\_methodology http://en.wikipedia.org/wiki/Rosenbrock function http://en.wikipedia.org/wiki/Sampling\_(statistics) http://en.wikipedia.org/wiki/Search\_algorithm http://en.wikipedia.org/wiki/Second\_derivative\_test http://en.wikipedia.org/wiki/Sensitivity analysis http://en.wikipedia.org/wiki/Sequential\_quadratic\_programming http://en.wikipedia.org/wiki/Simplex\_algorithm http://en.wikipedia.org/wiki/Simulated\_annealing http://en.wikipedia.org/wiki/Stochastic\_gradient\_descent http://en.wikipedia.org/wiki/Stochastic\_hill\_climbing http://en.wikipedia.org/wiki/Stochastic optimization http://en.wikipedia.org/wiki/Swarm\_intelligence http://en.wikipedia.org/wiki/Symbolic differentiation http://en.wikipedia.org/wiki/Uncertainty\_quantification

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# Appendix 7: Plug and Play Component Modeling — The CSDMS2.0 Approach

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**Abstract:** The CSDMS2.0 focus is on developing a software modelling environment that offers the earth and ocean communities products to enable easier penetration into the world of high performance computing, plug-and-play component modelling, and access to vetted open source surface-dynamics models. Protocols and standards define modelling interfaces, standard names, service components, and DOIs labelling.

Keywords: Semantic mediation; model framework; model coupling.

#### 1. INTRODUCTION

The Community Surface Dynamics Modeling System, or CSDMS, develops, integrates, archives and disseminates software to define the earth's surface dynamics. CSDMS coordinates a large (67 country) international community in building a toolbox of surface dynamics component models. The challenge encapsulates the variety of users, the volunteer effort, and the hundreds of very different models. The CSDMS Integration Facility develops the cyber-architecture and framework, to populate a plug-and-play component-modeling environment, able to operate within a cloud-sourced High Performance Computing environment.

#### 2. WMT: THE CSDMS WEB MODELING TOOL

The CSDMS Web Modeling Tool (WMT) is the web-based successor to the desktop Component Modeling Tool (Peckham et al., 2013). WMT provides a client-side drag-and-drop graphical interface and a server-side database and application programming interface (API) that allows users to build and run coupled surface dynamics models on a high-performance computing cluster (HPCC) from a web browser on a desktop, laptop or tablet computer. With WMT, a user can:

- Select a component model from a list to run in standalone mode,
- Build a coupled model from multiple components organized as nodes of a tree structure,
- View and edit the parameters for these model components,
- Upload custom input files to the server,
- Save models to a server, where they can be accessed on any Internet-accessible computer,
- Share saved models with others in the community, and
- Run a model by connecting to a remote HPCC where the components are installed.

Although WMT is web-based, the building and configuration of a model can be done offline. Reconnection is necessary only when saving a model and submitting it for a run.

#### 2.1 Client Overview

WMT presents a streamlined graphical interface, consisting of three scrollable panels, or views, and one menu (Fig. 1).

- *Components view* a list of Common Component Architecture (CCA) components (Armstrong et al., 1999) that is available on the HPCC.
- *Model view* a component can be dragged from the Components view into the tree structure of the Model view. Once in the tree, the component displays its CCA uses ports as leaves on the tree, i.e. a hierarchical form based on model component data requirements. By adding other components that provide ports for these open leaves, a coupled model can be created. A component instance that provides feedback to the coupled model is displayed as a link (e.g. CEM in Fig. 1).
- *Parameters view* displays model parameters in the Model view for viewing and editing. Type and range checks are performed immediately on any parameter that is modified.

Model menu — provides selections for opening, closing, saving, deleting and running models. Models developed
with WMT are currently saved to a server at CSDMS. When a model run is initiated, the user is provided with a
list of available HPCC nodes on which it can be run, and prompted to provide login credentials for the selected
HPCC.



Figure 1. The WMT client, showing the construction of a coupled model.

A model run can be initiated and its status (uploaded, staged, launched, complete) viewed; on completion, the model output can be retrieved by FTP.

#### 2.2 Client Architecture

The WMT client is written with GWT (GWT Project, 2013), a toolkit for building browser-based applications. Using GWT over native JavaScript offers the advantage that the client code is written in Java, which allows the developer to employ object-oriented design principles and mature Java development tools such as Eclipse. GWT provides a development mode for rapid prototyping and debugging, and a production mode, where the Java source is compiled to JavaScript for deployment on the web. GWT is used in several Google projects, and boasts a large user community. GWT is supported on all modern browsers, including Firefox, Internet Explorer (6+), Safari (5+), Chromium/Chrome and Opera. The WMT client uses the model-view-presenter (MVP) pattern (Fowler, 2006):

- *Model*: The layer providing data for the application.
- View. The user interface for viewing and modifying the application data (Fig. 2).
- *Presenter*. The mediator between the Model and the View. Messages are passed between View and Presenter, and between Model and Presenter, but the View and Model are designed to have no knowledge of the other.

MVP architecture separates the domain logic of an application, where rules are set for how data are stored and modified, from the client interface, where the user can interact with the data. This separation of responsibilities makes it easier to test, modify and maintain an application. MVP is particularly useful in applications that have a graphical user interface, since the testing of the interface often must be done manually (Wellman, 2008). The GWT Project recommends MVP for GWT applications (GWT Project, 2010).



Figure 2. The Model-View-Presenter (MVP) architecture pattern is adapted from Wellman (2008).

#### 2.3 Server Overview

The WMT server is a RESTful (Fielding, 2000) web application that provides a uniform interface through which client applications interact with the CSDMS model-coupling framework. Although opaque to a client, behind the WMT server is a layered system that consists of the following resources:

- A database server that contains component, model, and simulation metadata
- One or more execution servers on which simulations are launched
- A data server on which simulation output is stored and from which it can be downloaded.

The database server provides, as JSON encoded messages, the component metadata necessary for an end-user to couple components, and set input parameters. The metadata includes descriptions of component exchange items, uses and provides ports, as well as user-modifiable input parameters. It is held on a server separate from the execution server so that it is easily and quickly accessed without need to connect to a firewalled or inaccessible execution server. Execution servers are computational resources that contain the software stack needed to run a coupled or uncoupled model simulation. These servers can range from large high performance computing clusters, to smaller web servers, or even to an end-user's personal computer. The requirements are only that the WMT server has network access to the execution server and that the CSDMS software stack is installed on the server. This includes the CCA-toolchain, the CSDMS framework tools, and compiled shared libraries for each of the component models. Once a simulation completes, its output is packaged and uploaded to a data server where it is stored and from which the end-user is able to download it as a single compressed archive file.

#### 2.4 Incorporating BMI Models into the CSDMS Modeling Framework

The CSDMS Basic Modeling Interface (BMI) specification (Peckham et al., 2013) describes an application-programming interface (API) for scientific numerical models. The interface identifies entry points into software components to provide a calling application with the necessary level of control over the components that is necessary for two-way model coupling. CSDMS as well as other modeling frameworks, such as ESMF (Hill et al., 2004), OpenMI (Gregerson, 2007), and OMS (David et al., 2002), have identified the minimum granularity of control to be an interface that provides functionality to initialize, update, and finalize a component model. BMI establishes precise names, calling signature and return types for each of these functions in a language agnostic manner and also provides bindings for each of the CSDMS supported languages (Python, C, C++, Fortran, Java). Because modeling-coupling frameworks, not just the CSDMS model-coupling framework.

A component model that strictly follows the BMI specification allows for a streamlined workflow that enables it to function inside the CSDMS model-coupling framework. Templates exist for each supported language, and consists of boilerplate code that makes functions calls to CSDMS and CCA services but will only access the underlying component model through BMI function calls. Wrapper templates will never make reference to component-specific functions or

data. Rather, component control (initialize, update, finalize) and data access (getters, setters) is always through BMI functions. Then, at run-time, these function references are linked dynamically to the shared library that contains the compiled BMI implementation for the appropriate component. BMI functions provide most component metadata (names of input / output exchange items). Additional metadata the CSDMS framework needs to incorporate a new component include:

- Source code: author(s), license, version, link to source code, etc.
- Input files: File templates that contain placeholders for adjustable parameters
- Input parameters: description of user-adjustable input parameters

These additional source code metadata provide end users with standardized model information. If a component requires input files to operate, the component contributor must provide template versions of these files. Additionally, if the contributor would like some of these parameters to be editable by an end user, the template files should include placeholders for the adjustable parameters. A placeholder is simply a key name, which refers to the parameter, enclosed in curly-braces. Each input parameters must be described (float, int, string, etc.), along with suggested ranges, and a short description of the parameter. This additional metadata is used by various CSDMS tools to enhance the end-user experience and help overcome the "black-box syndrome" that results from users running models without being aware of the model's inner workings.

#### 3. CSDMS STANDARD NAMES AND MODEL METADATA

In order to develop a modeling framework that would allow automated coupling of models and data sets from different contributors, semantic mediation or matching is required. Each model and data set uses its own terms or labels for input and output variable names, often domain-specific or abbreviated. To ensure that one model's output variable is appropriate for use as another model's input, a precise description of the variable, its units and certain other attributes are required. To address this need, a semantic matching called the CSDMS Standard Names was developed. These standardized names avoid domain-specific terms and abbreviations, are based on a set of rules or conventions and are designed to eliminate ambiguity. Contributors of models or data sets are asked to map each of their own terms to the appropriate "long name" in the CSDMS Standard Names. For models or data sets, this can be done by implementing a CSDMS Basic Model Interface (BMI) that provides standardized self-description as well as model control functions (i.e. initialize, update, finalize). The model control functions provide the modeling framework with fine-grained control of the model and allow heterogeneous models to be coupled within the CSDMS framework. Contributors create the mapping (e.g. Python dictionary) from their model's internal variable names to CSDMS standard names, and supply information about the spatial grid, time-stepping scheme, and assumptions.

The CSDMS Standard Names are unique labels for model variables that are not specific to any particular modeling domain. CSDMS Standard Names for variables always consist of an object part and a quantity/attribute part and the quantity part may have an operation prefix that can consist of multiple operations. Unlike the CF Standard Names, assumptions and explanations are not included in the name itself; they are instead selected from a standardized list and specified with <assume> tags in a Model Metadata File (XML) that clarifies how a given model uses the name. CSDMS Standard Names consist of Model Variable Names and Model Metadata Names. Model Variable names are constructed from valid Object Names, Operation Names and Quantity Names. Quantity Names often include a Process Name. Model Metadata Names attempt to provide complete metadata for describing key attributes of a model other than the input and output variable names and are stored in Model Metadata Files. Model Metadata Names include additional metadata to support the variable names, such as units, object name source and geo-referencing data (e.g. standard ellipsoid, datum and projection names) and different types of Assumption Names. For further detail, readers are referred to <u>http://csdms.colorado.edu/wiki/CSDMS\_Standard\_Names</u>. Developers continue to use whatever variable names they want to in their model code or data set, but must then "map" each of their internal variable names to the appropriate CSDMS standard name in their BMI implementation.

The standard names used in the CEM-Avulsion coupling (Fig. 1) would see HydroTrend provide to Avulsion:

- channel\_outflow\_end\_water\_\_speed
- channel\_outflow\_end\_\_width
- channel\_outflow\_end\_water\_\_depth
- channel\_outflow\_end\_water\_\_discharge
- channel\_outflow\_end\_suspended\_sediment\_\_discharge

• channel\_outflow\_end\_bed\_load\_sediment\_\_mass\_flow\_rate

*Waves* provides to *CEM*:

- sea\_water\_surface\_wave\_\_height
- sea\_water\_surface\_wave\_period

Avulsion provides to CEM:

- channel\_outflow\_end\_bed\_load\_sediment\_\_mass\_flow\_rate
- channel\_outflow\_end\_water\_\_discharge
- channel\_outflow\_end\_\_location\_model\_x\_component
- channel\_outflow\_end\_location\_model\_y\_component

CEM provides to Avulsion:

• land\_surface\_\_elevation

#### 4. CSDMS SERVICE COMPONENTS

CSDMS employs two versions of ESMF regridding tools, in combination with CSDMS **regridding tools**. The serial version is used on single-processor platforms; Message Passing Interface (MPI) is employed for use with multiple processors. The parallel version of the mapper scales nearly linearly up to several dozen processors. These mappers map elements from one unstructured grid to another. While grid elements are typically either three or four sided, ESMF offers a more general tool that supports polygonal cells with an arbitrary number of sides. This makes it possible for a model that uses watershed polygons as its "computational cells" to obtain spatially interpolated rainfall data from a data source that uses rectangular cells.

Earth surface process models may use fixed or adaptive time-stepping schemes, and coupled models may use time-steps that are significantly different in size. A snowmelt model may employ hourly time-steps and be coupled to a channelized flow model that uses time-steps of several seconds. "Temporal misalignment" may have unintended consequences. Application of a smooth interpolation function to each of the state variables in the model with the larger time-step allows the smaller time-step model to retrieve and use interpolated values that vary more smoothly and which can be updated (with every time-step) with very low computational cost. A new time **interpolation service component** is made available to components run through the CSDMS WMT framework.

CSDMS has created **file-writing tools** for use within the CSDMS framework. The new writer class receives data from a component model and outputs the data to either a VTK file or a NetCDF file. VTK files are written in binary using the "new-style" XML format for VTKs. For structured grids, NetCDF files follow the CF conventions. For storing unstructured (flexible) meshes in NetCDF format, we employ the UGRID standard (<u>https://github.com/ugrid-conventions</u>).

#### 5. BEYOND THE BLACK BOX MODEL

A "black box" model can be manipulated in terms of its input and then generates output for a user without having knowledge of its internal workings or without being able to get insight in the model engine, or its process routines. The model algorithms and their implementation are then "opaque" or "black". CSDMS strives to take models and components beyond black box state. Science practice in principle condemns a "black box"; it is of crucial importance to know the level of process simplification within a model engine and the implementation into equations and a numerical scheme. Without such transparency the analysis of model output is of much less value.

CSDMS also offers web-based metadata on each model, submitted by the original developers, and maintained as a wiki database and thus updatable by users themselves. CSDMS maintains an online model repository where the original code can be downloaded, viewed, compiled and run. The model engines are thus available to any user. WMT components are documented in more detail on the CSDMS wiki (Figs. 3 and 4). With WMT, a user can access: 1) more extensive model description, 2) notes on input parameters, 3) key model equations, 4) notes on coupling ports, and 5) essential references provided by the original developer.

Pedagogical research shows the importance of hands-on activities in learning (Campbell et al., 2013). Students show significant learning gains when they work with inquiry-based modules and receive instantaneous feedback (Fogleman et al., 2011). The CSDMS Educational Working Group noted that hands-on modeling labs are more valuable if they are combined with mathematical and physics problems based on the careful analysis of the underlying model engine (Schwarz et al., 2009). CSDMS offers an educational repository with modeling labs for graduate and advanced undergraduate students. These labs support students to run models, analyze output and highlight some critical aspect of the modeled processes and model engine, the selection of which depend on the learning objective and lesson plan.



Figure 3. All components in the WMT have live links to online detailed documentation maintained on the CSDMS wiki.



Figure 4. Detailed model description of the CEM-Coastline Evolution Model as displayed within WMT.

#### 6. DIGITAL OBJECT IDENTIFIERS FOR NUMERICAL MODELS

All code in CSDMS is open source (see Ince et al., 2012). Source code exposes the scientific hypotheses embodied in a numerical model, and the solution to the set of equations. Code transparency allows for full peer review and replication of results — the foundation of modern science. Code transparency allows for reuse in new and clever ways, and reduces redundancy. CSDMS ensures that model developers receive recognition for their work, even when code is submitted and not yet described in a scientific journal by adopting the Digital Object Identifier (DOI). The DOI system provides a unique identification to content that is available on digital networks. Since 2005 DOIs were made available for research data (Paskin, 2005). CSDMS is the first to assign Digital Object Identifiers (DOIs) to numerical source code. The advantages of adopting a DOI system for models include:

- Guarantee credit to a model developer.
- Reuse and replication of research with direct access to a referenced code.
- Higher visibility content with a DOI is 5 times more likely to deliver active links.

• The opportunity for funding agencies to track usage, so to measure impact.

CSDMS collaborates with Integrated Earth Data Applications (IEDA), a formal Publication Agent of the DOI system through the German National Library of Science and Technology, to assign unique identifiers for those models that contain metadata and are physically part of the CSDMS repository. An archive of all numerical models of the CSDMS model repository that have a DOI, together with limited metadata and source code is provided to IEDA to guaranty access beyond the CSDMS program; a DOI for an object is permanent, whereas its location and other metadata may change in future. A new DOI is provided for each new version of a model (i.e. major upgrade/version of the source code). CSDMS uses Apache Subversion, better known as SVN, for tracking source code versioning and revision control so that current and past releases and changes can be accessed through the web. As of March 2014, 109 models within the CSDMS model repository have a DOI. Model source code can be viewed as 'data' and therefore CSDMS endorses citations defined by DataCite guidelines (Brase, 2010). Following these guidelines, CSDMS strongly recommends the following structure for citing a model: *ModelDeveloper (PublicationYear). ModelName, ModelVersion. Identifier.* 

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